



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 11:45 PM EST

PDB ID : 2MU3
BMRB ID : 17899
Title : Spider wrapping silk fibre architecture arising from its modular soluble protein precursor
Authors : Xu, L.; Tremblay, M.; Meng, Q.; Liu, X.; Rainey, J.K.; Lefevre, T.; Sarker, M.; Orrell, K.E.; Leclerc, J.; Pezolet, M.; Auger, M.
Deposited on : 2014-09-03

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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

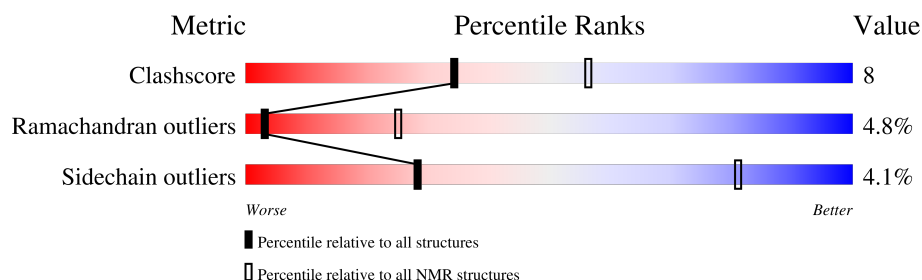
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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 | 210492 | 14027 |
| Ramachandran outliers | 207382 | 12486 |
| Sidechain outliers | 206894 | 12463 |

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 | 199 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|--------------------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:12-A:77, A:86-A:144 (125) | 0.92 | 18 |

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 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2632 atoms, of which 1296 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Aciniform spidroin 1.

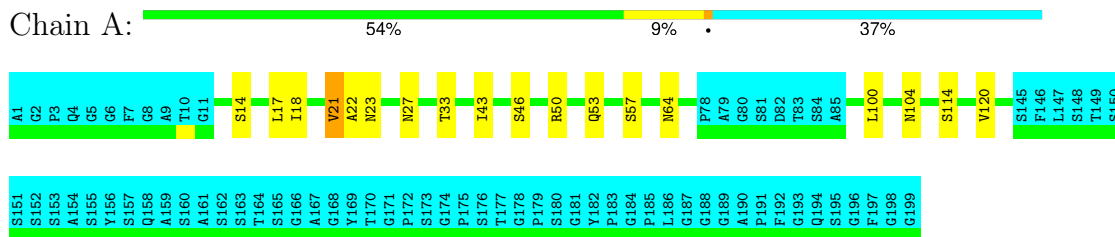
| Mol | Chain | Residues | Atoms | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|-------|
| 1 | A | 199 | Total | C | H | N | O | 0 |
| | | | 2632 | 809 | 1296 | 240 | 287 | |

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: Aciniform spidroin 1

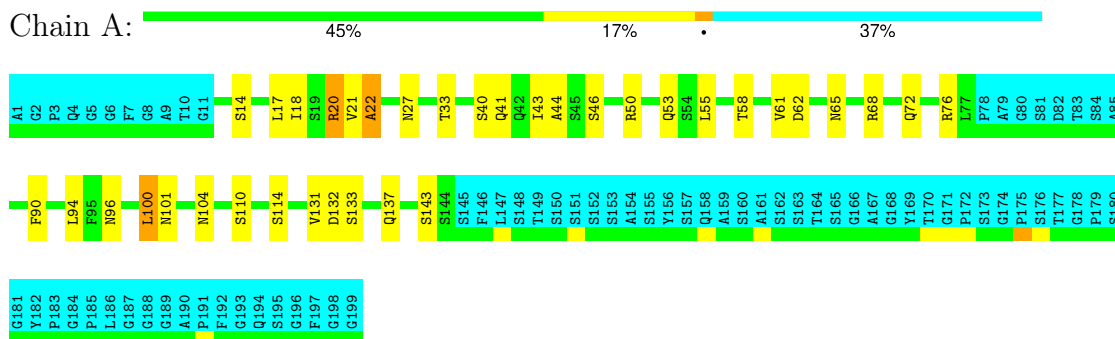


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

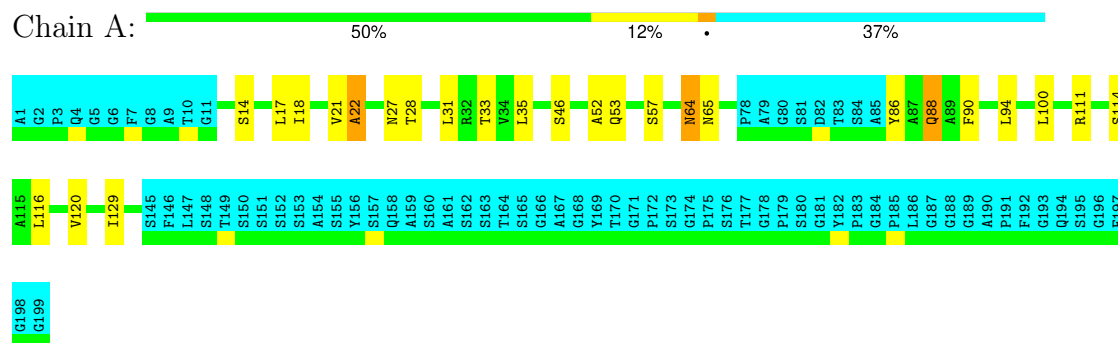
4.2.1 Score per residue for model 1

- Molecule 1: Aciniform spidroin 1



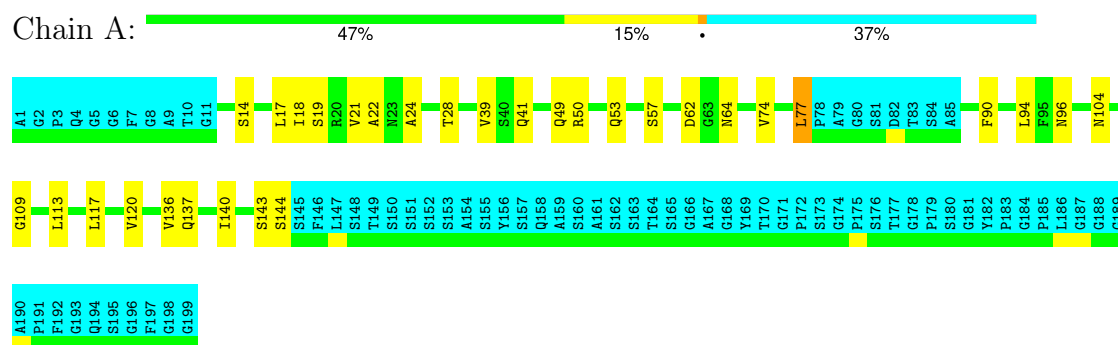
4.2.2 Score per residue for model 2

- Molecule 1: Aciniform spidroin 1



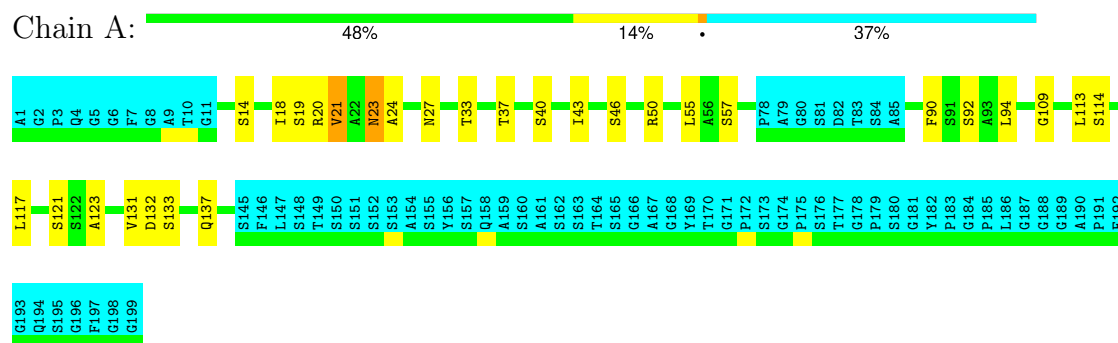
4.2.3 Score per residue for model 3

- Molecule 1: Aciniform spidroin 1



4.2.4 Score per residue for model 4

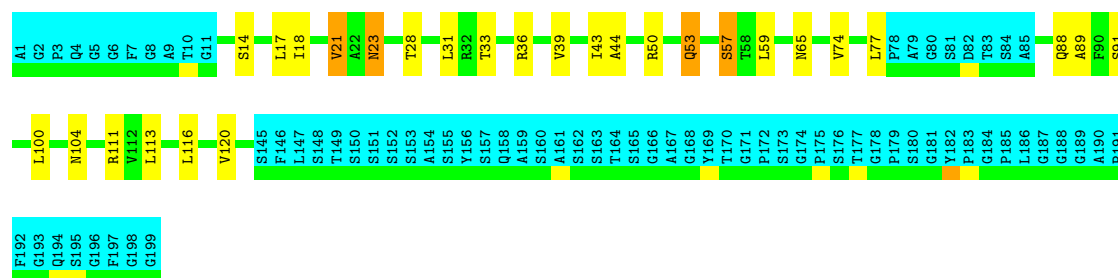
- Molecule 1: Aciniform spidroin 1



4.2.5 Score per residue for model 5

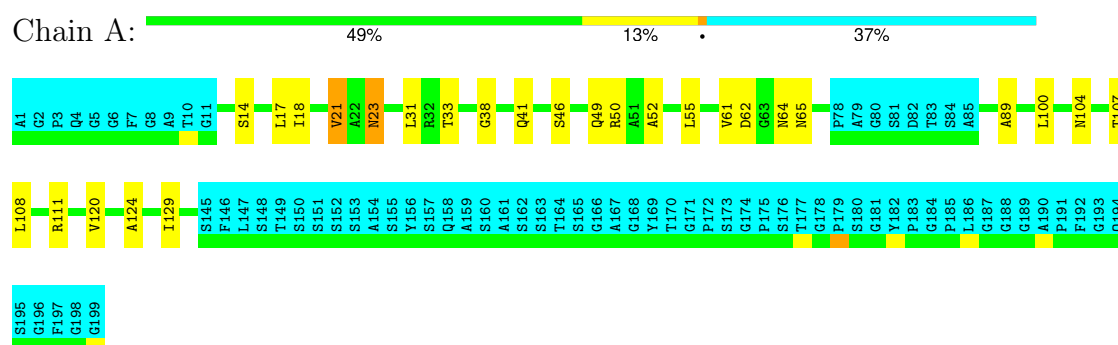
- Molecule 1: Aciniform spidroin 1





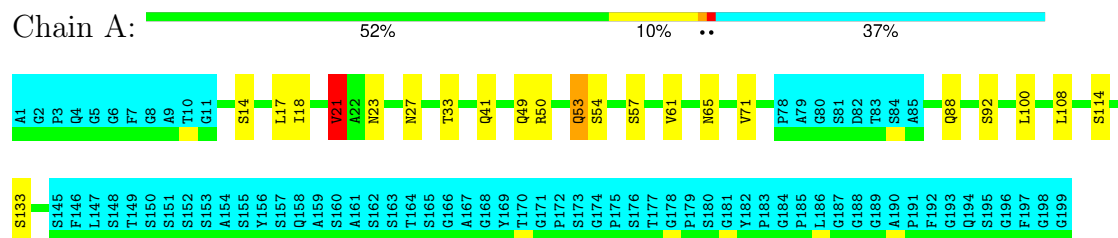
4.2.6 Score per residue for model 6

- Molecule 1: Aciniform spidroin 1



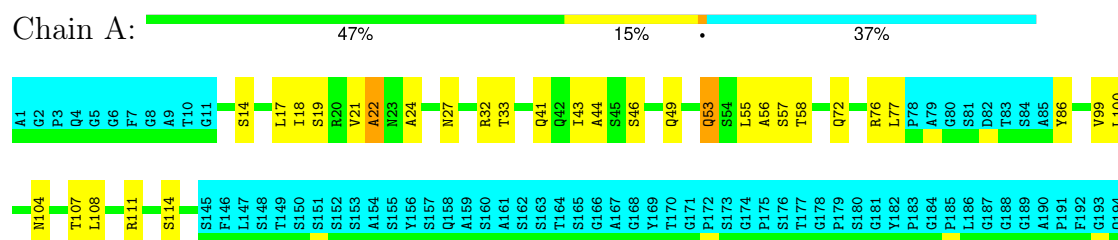
4.2.7 Score per residue for model 7

- Molecule 1: Aciniform spidroin 1



4.2.8 Score per residue for model 8

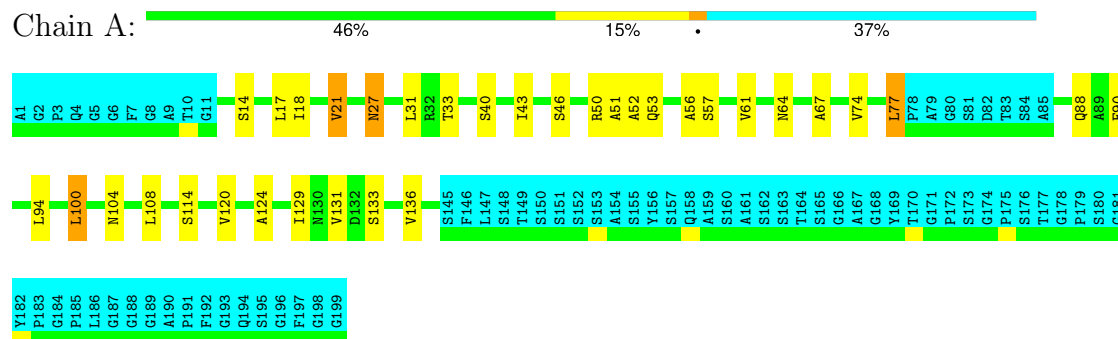
- Molecule 1: Aciniform spidroin 1



S195
G196
F197
G198
G199

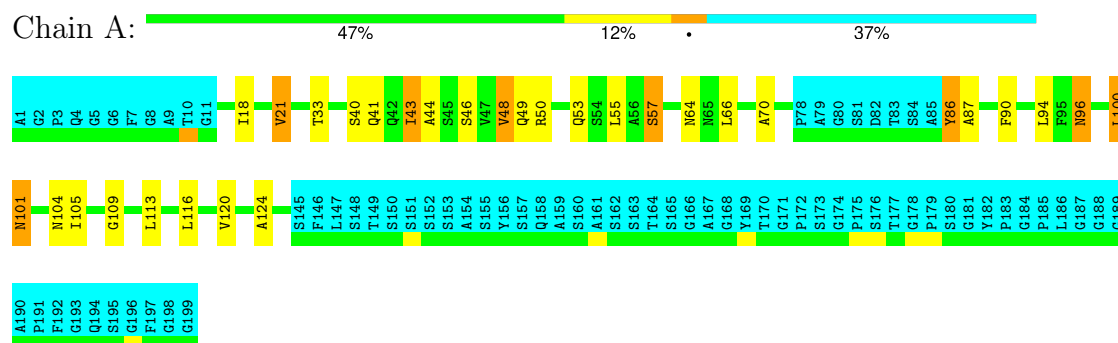
4.2.9 Score per residue for model 9

- Molecule 1: Aciniform spidroin 1



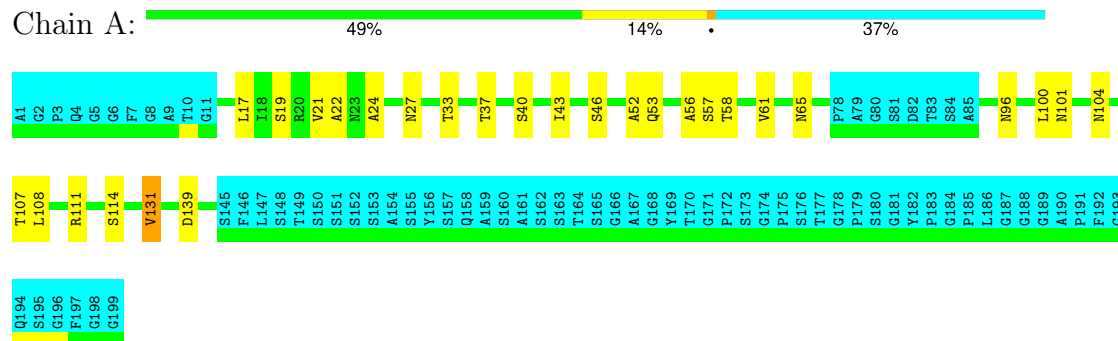
4.2.10 Score per residue for model 10

- Molecule 1: Aciniform spidroin 1



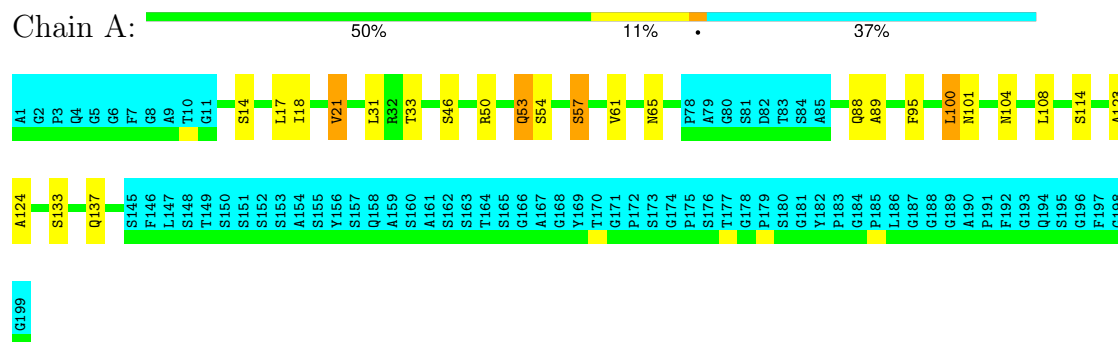
4.2.11 Score per residue for model 11

- Molecule 1: Aciniform spidroin 1



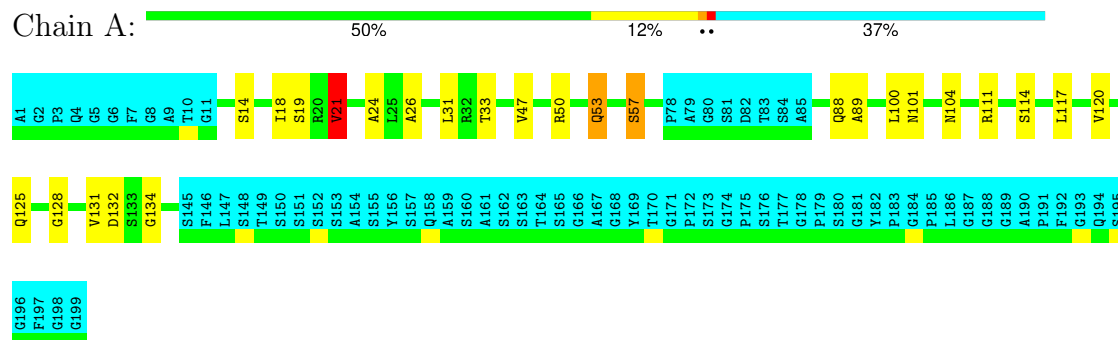
4.2.12 Score per residue for model 12

- Molecule 1: Aciniform spidroin 1



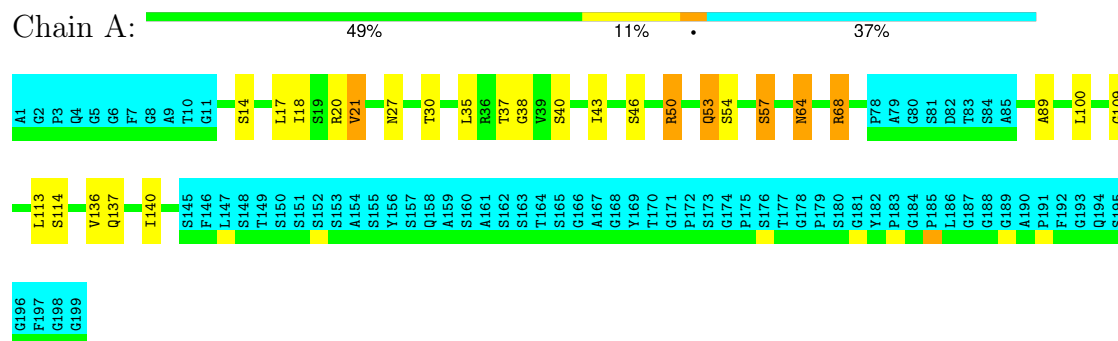
4.2.13 Score per residue for model 13

- Molecule 1: Aciniform spidroin 1



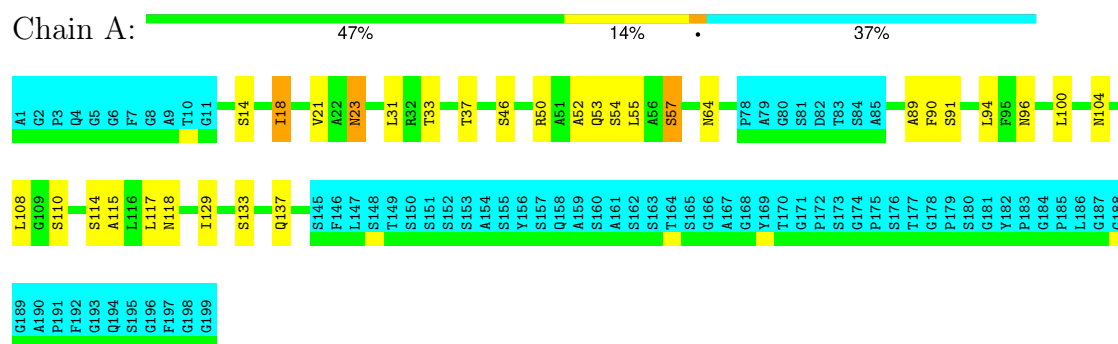
4.2.14 Score per residue for model 14

- Molecule 1: Aciniform spidroin 1



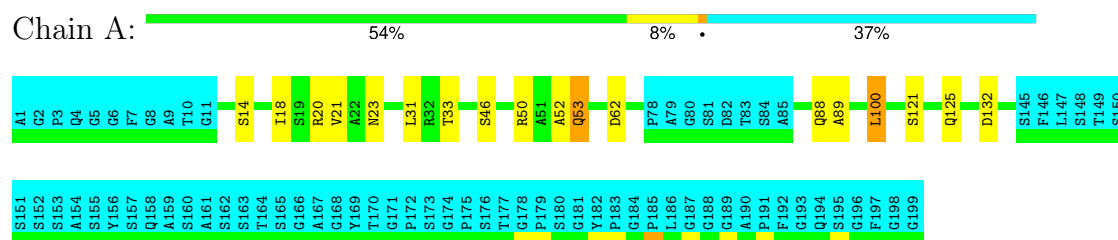
4.2.15 Score per residue for model 15

- Molecule 1: Aciniform spidroin 1



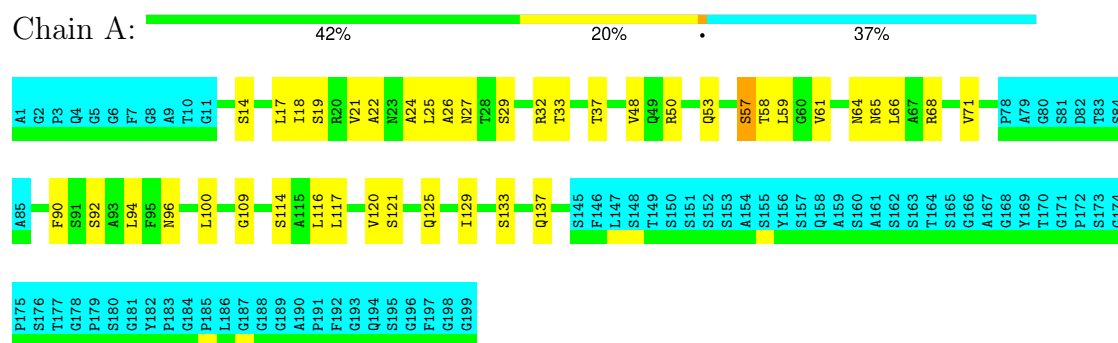
4.2.16 Score per residue for model 16

- Molecule 1: Aciniform spidroin 1



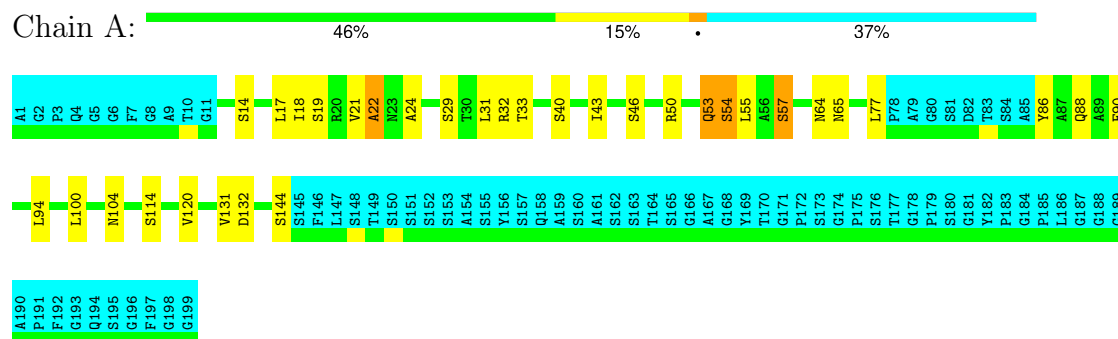
4.2.17 Score per residue for model 17

- Molecule 1: Aciniform spidroin 1



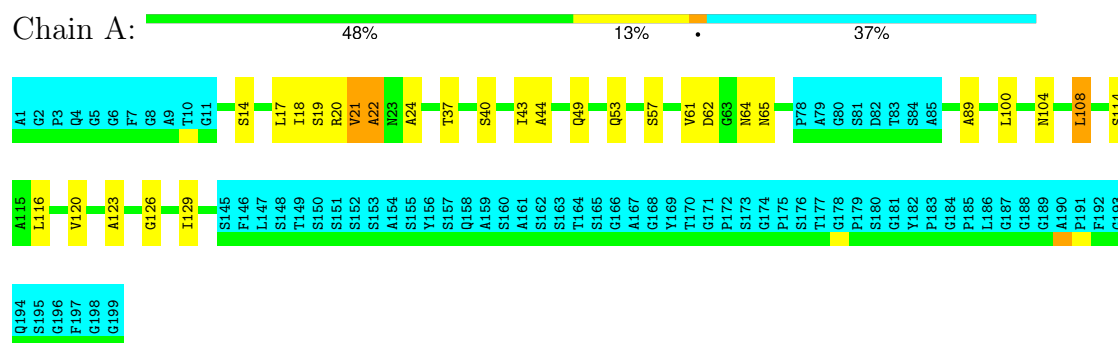
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Aciniform spidroin 1



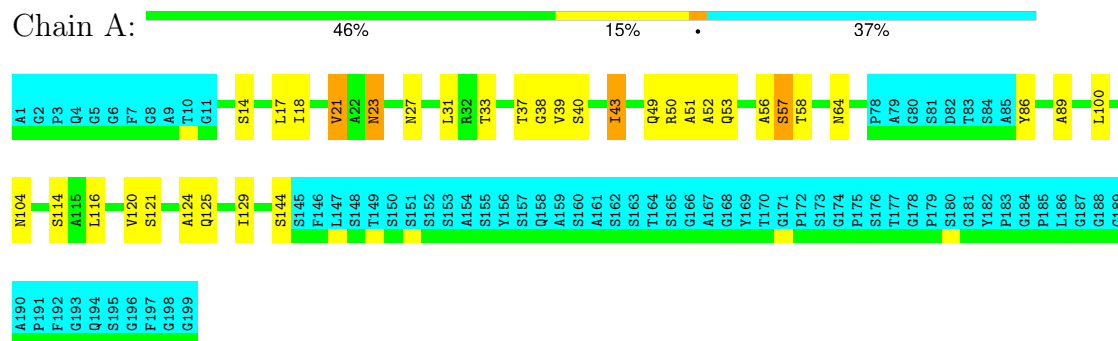
4.2.19 Score per residue for model 19

- Molecule 1: Aciniform spidroin 1



4.2.20 Score per residue for model 20

- Molecule 1: Aciniform spidroin 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| NMRPipe | refinement | 1.0 |
| NMRPipe | refinement | 1.0 |
| NMRPipe | refinement | 1.0 |
| NMRPipe | refinement | 1.0 |
| NMRPipe | refinement | 1.0 |
| NMRPipe | refinement | 1.0 |
| ARIA | refinement | 2 |
| ARIA | structure solution | 2 |
| X-PLOR NIH | 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 | 2015 |
| Number of shifts mapped to atoms | 2015 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 91% |

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 | 873 | 888 | 888 | 14±4 |
| All | All | 17460 | 17760 | 17760 | 277 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:52:ALA:HB2 | 1:A:129:ILE:HG23 | 0.66 | 1.67 | 6 | 3 |
| 1:A:61:VAL:HA | 1:A:65:ASN:OD1 | 0.63 | 1.93 | 1 | 7 |
| 1:A:43:ILE:HG13 | 1:A:44:ALA:N | 0.62 | 2.09 | 5 | 2 |
| 1:A:59:LEU:HD11 | 1:A:65:ASN:ND2 | 0.62 | 2.09 | 5 | 1 |
| 1:A:50:ARG:NH1 | 1:A:123:ALA:HA | 0.61 | 2.10 | 12 | 1 |
| 1:A:53:GLN:HB3 | 1:A:61:VAL:O | 0.60 | 1.96 | 7 | 1 |
| 1:A:53:GLN:O | 1:A:57:SER:HB2 | 0.58 | 1.98 | 5 | 13 |
| 1:A:40:SER:HA | 1:A:49:GLN:O | 0.58 | 1.97 | 20 | 3 |
| 1:A:117:LEU:HA | 1:A:120:VAL:HG22 | 0.57 | 1.75 | 13 | 1 |
| 1:A:38:GLY:HA3 | 1:A:129:ILE:HG21 | 0.57 | 1.76 | 6 | 1 |
| 1:A:21:VAL:HG11 | 1:A:100:LEU:HB3 | 0.57 | 1.77 | 12 | 4 |
| 1:A:17:LEU:O | 1:A:21:VAL:HG23 | 0.56 | 2.01 | 2 | 14 |
| 1:A:100:LEU:HD23 | 1:A:100:LEU:H | 0.56 | 1.60 | 5 | 1 |
| 1:A:77:LEU:HB3 | 1:A:86:TYR:OH | 0.55 | 2.01 | 18 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:100:LEU:H | 1:A:100:LEU:HD23 | 0.55 | 1.60 | 6 | 6 |
| 1:A:50:ARG:CZ | 1:A:55:LEU:HD22 | 0.55 | 2.32 | 10 | 1 |
| 1:A:14:SER:O | 1:A:18:ILE:HG23 | 0.54 | 2.02 | 18 | 18 |
| 1:A:18:ILE:HB | 1:A:89:ALA:O | 0.54 | 2.02 | 12 | 8 |
| 1:A:38:GLY:CA | 1:A:129:ILE:HG21 | 0.54 | 2.32 | 6 | 1 |
| 1:A:39:VAL:O | 1:A:50:ARG:HA | 0.54 | 2.03 | 5 | 2 |
| 1:A:50:ARG:O | 1:A:50:ARG:HG2 | 0.53 | 2.04 | 1 | 2 |
| 1:A:31:LEU:HD23 | 1:A:31:LEU:H | 0.53 | 1.64 | 5 | 2 |
| 1:A:38:GLY:HA2 | 1:A:50:ARG:O | 0.53 | 2.04 | 20 | 2 |
| 1:A:43:ILE:H | 1:A:43:ILE:HD13 | 0.53 | 1.64 | 20 | 1 |
| 1:A:53:GLN:HG2 | 1:A:61:VAL:O | 0.52 | 2.04 | 9 | 1 |
| 1:A:17:LEU:O | 1:A:21:VAL:HG22 | 0.52 | 2.04 | 7 | 1 |
| 1:A:28:THR:HA | 1:A:143:SER:OG | 0.52 | 2.04 | 3 | 1 |
| 1:A:107:THR:O | 1:A:111:ARG:HD2 | 0.52 | 2.05 | 6 | 1 |
| 1:A:19:SER:O | 1:A:24:ALA:HB2 | 0.51 | 2.05 | 4 | 8 |
| 1:A:31:LEU:H | 1:A:31:LEU:HD23 | 0.51 | 1.66 | 2 | 2 |
| 1:A:40:SER:O | 1:A:43:ILE:HG13 | 0.51 | 2.06 | 4 | 6 |
| 1:A:53:GLN:CD | 1:A:53:GLN:H | 0.51 | 2.09 | 7 | 3 |
| 1:A:31:LEU:HA | 1:A:88:GLN:O | 0.51 | 2.06 | 16 | 5 |
| 1:A:53:GLN:H | 1:A:53:GLN:CD | 0.51 | 2.09 | 17 | 3 |
| 1:A:96:ASN:O | 1:A:100:LEU:HD22 | 0.50 | 2.06 | 17 | 1 |
| 1:A:21:VAL:HG12 | 1:A:22:ALA:N | 0.50 | 2.22 | 11 | 7 |
| 1:A:50:ARG:NH1 | 1:A:55:LEU:HD13 | 0.50 | 2.21 | 18 | 1 |
| 1:A:107:THR:O | 1:A:111:ARG:HD3 | 0.50 | 2.07 | 11 | 2 |
| 1:A:49:GLN:OE1 | 1:A:58:THR:HB | 0.49 | 2.06 | 20 | 1 |
| 1:A:115:ALA:HA | 1:A:118:ASN:ND2 | 0.49 | 2.23 | 15 | 1 |
| 1:A:29:SER:HA | 1:A:32:ARG:HB3 | 0.49 | 1.84 | 18 | 2 |
| 1:A:90:PHE:O | 1:A:94:LEU:HG | 0.49 | 2.07 | 10 | 9 |
| 1:A:94:LEU:O | 1:A:120:VAL:HG11 | 0.49 | 2.08 | 3 | 3 |
| 1:A:74:VAL:O | 1:A:77:LEU:HD22 | 0.49 | 2.07 | 9 | 1 |
| 1:A:101:ASN:O | 1:A:104:ASN:HB3 | 0.48 | 2.08 | 1 | 3 |
| 1:A:43:ILE:HD11 | 1:A:86:TYR:CD1 | 0.48 | 2.42 | 10 | 1 |
| 1:A:116:LEU:O | 1:A:120:VAL:HG23 | 0.48 | 2.08 | 20 | 6 |
| 1:A:53:GLN:NE2 | 1:A:53:GLN:H | 0.48 | 2.06 | 5 | 2 |
| 1:A:86:TYR:HD1 | 1:A:87:ALA:N | 0.48 | 2.06 | 10 | 1 |
| 1:A:20:ARG:N | 1:A:20:ARG:HD2 | 0.48 | 2.23 | 1 | 1 |
| 1:A:48:VAL:HG22 | 1:A:70:ALA:HB1 | 0.48 | 1.85 | 10 | 1 |
| 1:A:21:VAL:HG13 | 1:A:100:LEU:HB3 | 0.48 | 1.85 | 19 | 3 |
| 1:A:68:ARG:HA | 1:A:72:GLN:NE2 | 0.48 | 2.24 | 1 | 1 |
| 1:A:133:SER:HA | 1:A:137:GLN:CB | 0.48 | 2.39 | 1 | 3 |
| 1:A:50:ARG:NH2 | 1:A:54:SER:HB3 | 0.48 | 2.24 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:51:ALA:HB3 | 1:A:131:VAL:HG12 | 0.47 | 1.87 | 9 | 1 |
| 1:A:104:ASN:O | 1:A:108:LEU:HG | 0.47 | 2.09 | 8 | 3 |
| 1:A:21:VAL:HG11 | 1:A:100:LEU:CB | 0.47 | 2.40 | 20 | 6 |
| 1:A:43:ILE:HG13 | 1:A:44:ALA:H | 0.47 | 1.68 | 5 | 1 |
| 1:A:23:ASN:HB3 | 1:A:31:LEU:HD22 | 0.47 | 1.87 | 20 | 3 |
| 1:A:64:ASN:HA | 1:A:68:ARG:NH2 | 0.46 | 2.25 | 14 | 1 |
| 1:A:136:VAL:O | 1:A:140:ILE:HG12 | 0.46 | 2.11 | 3 | 2 |
| 1:A:23:ASN:HB2 | 1:A:92:SER:OG | 0.46 | 2.10 | 4 | 1 |
| 1:A:133:SER:HA | 1:A:137:GLN:HB3 | 0.46 | 1.88 | 4 | 3 |
| 1:A:74:VAL:O | 1:A:77:LEU:HG | 0.46 | 2.10 | 5 | 1 |
| 1:A:37:THR:HB | 1:A:129:ILE:O | 0.46 | 2.11 | 19 | 1 |
| 1:A:120:VAL:HG13 | 1:A:124:ALA:HB3 | 0.46 | 1.88 | 10 | 3 |
| 1:A:21:VAL:HG12 | 1:A:22:ALA:H | 0.45 | 1.70 | 2 | 2 |
| 1:A:131:VAL:CG2 | 1:A:136:VAL:HG11 | 0.45 | 2.42 | 9 | 1 |
| 1:A:109:GLY:O | 1:A:113:LEU:HB2 | 0.44 | 2.12 | 14 | 3 |
| 1:A:74:VAL:O | 1:A:77:LEU:HD12 | 0.44 | 2.12 | 3 | 1 |
| 1:A:39:VAL:HG23 | 1:A:43:ILE:HD11 | 0.44 | 1.90 | 20 | 1 |
| 1:A:67:ALA:HA | 1:A:133:SER:O | 0.44 | 2.13 | 9 | 1 |
| 1:A:50:ARG:CZ | 1:A:55:LEU:HG | 0.44 | 2.42 | 6 | 1 |
| 1:A:104:ASN:O | 1:A:108:LEU:HD23 | 0.44 | 2.13 | 6 | 1 |
| 1:A:43:ILE:HD12 | 1:A:44:ALA:N | 0.44 | 2.27 | 19 | 2 |
| 1:A:52:ALA:CB | 1:A:129:ILE:HG23 | 0.44 | 2.43 | 9 | 1 |
| 1:A:18:ILE:HD12 | 1:A:89:ALA:O | 0.43 | 2.12 | 19 | 1 |
| 1:A:50:ARG:H | 1:A:56:ALA:HB2 | 0.43 | 1.72 | 9 | 1 |
| 1:A:50:ARG:HB2 | 1:A:55:LEU:HB2 | 0.43 | 1.88 | 15 | 1 |
| 1:A:110:SER:O | 1:A:114:SER:HA | 0.43 | 2.12 | 1 | 1 |
| 1:A:110:SER:HA | 1:A:117:LEU:HD12 | 0.43 | 1.89 | 15 | 1 |
| 1:A:77:LEU:HD13 | 1:A:86:TYR:CE2 | 0.43 | 2.48 | 8 | 1 |
| 1:A:41:GLN:HA | 1:A:44:ALA:HB3 | 0.43 | 1.90 | 10 | 1 |
| 1:A:49:GLN:HB2 | 1:A:56:ALA:HA | 0.43 | 1.90 | 8 | 2 |
| 1:A:35:LEU:HA | 1:A:88:GLN:CD | 0.43 | 2.34 | 2 | 1 |
| 1:A:109:GLY:CA | 1:A:117:LEU:HD12 | 0.43 | 2.43 | 3 | 2 |
| 1:A:27:ASN:HA | 1:A:32:ARG:NH2 | 0.43 | 2.29 | 8 | 1 |
| 1:A:72:GLN:O | 1:A:76:ARG:HG3 | 0.43 | 2.14 | 1 | 1 |
| 1:A:23:ASN:HB2 | 1:A:92:SER:CB | 0.42 | 2.44 | 7 | 1 |
| 1:A:95:PHE:O | 1:A:124:ALA:HB1 | 0.42 | 2.14 | 12 | 1 |
| 1:A:36:ARG:HB3 | 1:A:91:SER:OG | 0.42 | 2.15 | 5 | 1 |
| 1:A:43:ILE:HD13 | 1:A:44:ALA:N | 0.42 | 2.28 | 10 | 1 |
| 1:A:35:LEU:H | 1:A:35:LEU:HD23 | 0.42 | 1.74 | 14 | 1 |
| 1:A:58:THR:HG23 | 1:A:59:LEU:HG | 0.42 | 1.91 | 17 | 1 |
| 1:A:66:LEU:O | 1:A:71:VAL:HG23 | 0.42 | 2.14 | 17 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:VAL:CG1 | 1:A:22:ALA:N | 0.42 | 2.83 | 11 | 1 |
| 1:A:50:ARG:HE | 1:A:129:ILE:HG13 | 0.42 | 1.75 | 17 | 1 |
| 1:A:41:GLN:HB3 | 1:A:49:GLN:HA | 0.42 | 1.91 | 3 | 3 |
| 1:A:72:GLN:O | 1:A:76:ARG:HG2 | 0.42 | 2.14 | 8 | 1 |
| 1:A:50:ARG:HG2 | 1:A:50:ARG:O | 0.42 | 2.15 | 16 | 1 |
| 1:A:23:ASN:OD1 | 1:A:91:SER:HB3 | 0.41 | 2.14 | 15 | 1 |
| 1:A:64:ASN:CG | 1:A:65:ASN:H | 0.41 | 2.19 | 2 | 2 |
| 1:A:117:LEU:O | 1:A:121:SER:HB2 | 0.41 | 2.15 | 4 | 1 |
| 1:A:50:ARG:HH21 | 1:A:124:ALA:HB2 | 0.41 | 1.76 | 20 | 1 |
| 1:A:50:ARG:HD2 | 1:A:123:ALA:CB | 0.41 | 2.46 | 4 | 1 |
| 1:A:71:VAL:CG2 | 1:A:133:SER:HB2 | 0.41 | 2.45 | 7 | 1 |
| 1:A:101:ASN:ND2 | 1:A:104:ASN:HB3 | 0.41 | 2.31 | 10 | 1 |
| 1:A:131:VAL:HG12 | 1:A:132:ASP:H | 0.41 | 1.76 | 18 | 1 |
| 1:A:21:VAL:HB | 1:A:92:SER:HB3 | 0.41 | 1.91 | 17 | 1 |
| 1:A:121:SER:O | 1:A:125:GLN:HB3 | 0.41 | 2.15 | 20 | 1 |
| 1:A:131:VAL:HG12 | 1:A:132:ASP:N | 0.41 | 2.30 | 4 | 4 |
| 1:A:66:LEU:O | 1:A:70:ALA:HB3 | 0.41 | 2.15 | 10 | 1 |
| 1:A:14:SER:OG | 1:A:108:LEU:HD21 | 0.41 | 2.15 | 19 | 1 |
| 1:A:68:ARG:N | 1:A:68:ARG:HD2 | 0.41 | 2.31 | 17 | 1 |
| 1:A:55:LEU:O | 1:A:55:LEU:HD23 | 0.40 | 2.15 | 1 | 1 |
| 1:A:52:ALA:CB | 1:A:129:ILE:HG13 | 0.40 | 2.46 | 20 | 1 |
| 1:A:43:ILE:HD13 | 1:A:43:ILE:C | 0.40 | 2.36 | 10 | 1 |
| 1:A:56:ALA:O | 1:A:58:THR:N | 0.40 | 2.53 | 11 | 1 |
| 1:A:136:VAL:HG13 | 1:A:137:GLN:N | 0.40 | 2.31 | 3 | 1 |
| 1:A:50:ARG:HD3 | 1:A:55:LEU:HB3 | 0.40 | 1.92 | 4 | 1 |
| 1:A:121:SER:HA | 1:A:125:GLN:HB3 | 0.40 | 1.94 | 16 | 2 |
| 1:A:61:VAL:HG22 | 1:A:65:ASN:ND2 | 0.40 | 2.31 | 19 | 1 |
| 1:A:104:ASN:O | 1:A:108:LEU:HD13 | 0.40 | 2.16 | 19 | 1 |
| 1:A:51:ALA:N | 1:A:56:ALA:HB2 | 0.40 | 2.31 | 20 | 1 |
| 1:A:96:ASN:ND2 | 1:A:105:ILE:HG12 | 0.40 | 2.31 | 10 | 1 |
| 1:A:21:VAL:CG1 | 1:A:100:LEU:HB3 | 0.40 | 2.46 | 11 | 1 |

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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 | 125/199 (63%) | 96±3 (77±2%) | 23±3 (18±3%) | 6±2 (5±1%) | 3 | 25 |
| All | All | 2500/3980 (63%) | 1926 (77%) | 454 (18%) | 120 (5%) | 3 | 25 |

All 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 33 | THR | 17 |
| 1 | A | 114 | SER | 14 |
| 1 | A | 46 | SER | 13 |
| 1 | A | 57 | SER | 13 |
| 1 | A | 21 | VAL | 13 |
| 1 | A | 64 | ASN | 10 |
| 1 | A | 22 | ALA | 6 |
| 1 | A | 62 | ASP | 5 |
| 1 | A | 96 | ASN | 4 |
| 1 | A | 27 | ASN | 4 |
| 1 | A | 54 | SER | 4 |
| 1 | A | 58 | THR | 2 |
| 1 | A | 18 | ILE | 2 |
| 1 | A | 48 | VAL | 2 |
| 1 | A | 52 | ALA | 2 |
| 1 | A | 53 | GLN | 2 |
| 1 | A | 86 | TYR | 1 |
| 1 | A | 131 | VAL | 1 |
| 1 | A | 47 | VAL | 1 |
| 1 | A | 128 | GLY | 1 |
| 1 | A | 134 | GLY | 1 |
| 1 | A | 123 | ALA | 1 |
| 1 | A | 126 | GLY | 1 |

6.3.2 Protein sidechains ⓘ

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 | 94/139 (68%) | 90±1 (96±1%) | 4±1 (4±1%) | 28 | 81 |
| All | All | 1880/2780 (68%) | 1803 (96%) | 77 (4%) | 28 | 81 |

All 31 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 | 53 | GLN | 9 |
| 1 | A | 100 | LEU | 8 |
| 1 | A | 23 | ASN | 6 |
| 1 | A | 37 | THR | 6 |
| 1 | A | 104 | ASN | 5 |
| 1 | A | 27 | ASN | 4 |
| 1 | A | 108 | LEU | 4 |
| 1 | A | 111 | ARG | 3 |
| 1 | A | 21 | VAL | 3 |
| 1 | A | 41 | GLN | 2 |
| 1 | A | 28 | THR | 2 |
| 1 | A | 77 | LEU | 2 |
| 1 | A | 113 | LEU | 2 |
| 1 | A | 43 | ILE | 2 |
| 1 | A | 86 | TYR | 2 |
| 1 | A | 31 | LEU | 2 |
| 1 | A | 20 | ARG | 1 |
| 1 | A | 88 | GLN | 1 |
| 1 | A | 96 | ASN | 1 |
| 1 | A | 55 | LEU | 1 |
| 1 | A | 101 | ASN | 1 |
| 1 | A | 131 | VAL | 1 |
| 1 | A | 139 | ASP | 1 |
| 1 | A | 125 | GLN | 1 |
| 1 | A | 30 | THR | 1 |
| 1 | A | 50 | ARG | 1 |
| 1 | A | 68 | ARG | 1 |
| 1 | A | 137 | GLN | 1 |
| 1 | A | 132 | ASP | 1 |
| 1 | A | 25 | LEU | 1 |
| 1 | A | 54 | SER | 1 |

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

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 | 2015 |
| Number of shifts mapped to atoms | 2015 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 0 |

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 18 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 66 | LEU | HD11 | 0.917 | . | 2 |
| 1 | A | 66 | LEU | HD12 | 0.917 | . | 2 |
| 1 | A | 66 | LEU | HD13 | 0.917 | . | 2 |
| 1 | A | 21 | VAL | HG11 | 1.155 | 0.007 | 2 |
| 1 | A | 21 | VAL | HG12 | 1.155 | 0.007 | 2 |
| 1 | A | 21 | VAL | HG13 | 1.155 | 0.007 | 2 |
| 1 | A | 100 | LEU | HD11 | 0.597 | 0.004 | 2 |
| 1 | A | 100 | LEU | HD12 | 0.597 | 0.004 | 2 |
| 1 | A | 100 | LEU | HD13 | 0.597 | 0.004 | 2 |
| 1 | A | 117 | LEU | HD11 | 0.852 | 0.039 | 2 |
| 1 | A | 117 | LEU | HD12 | 0.852 | 0.039 | 2 |
| 1 | A | 117 | LEU | HD13 | 0.852 | 0.039 | 2 |
| 1 | A | 39 | VAL | HG11 | 1.164 | 0.013 | 2 |
| 1 | A | 39 | VAL | HG12 | 1.164 | 0.013 | 2 |
| 1 | A | 39 | VAL | HG13 | 1.164 | 0.013 | 2 |

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| List ID | Chain | Res | Type | Atom | Shift Data | | |
|---------|-------|-----|------|------|------------|-------------|-----------|
| | | | | | Value | Uncertainty | Ambiguity |
| 1 | A | 59 | LEU | HD11 | 0.740 | 0.013 | 2 |
| 1 | A | 59 | LEU | HD12 | 0.740 | 0.013 | 2 |
| 1 | A | 59 | LEU | HD13 | 0.740 | 0.013 | 2 |

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 |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 198 | -0.39 ± 0.07 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 164 | 0.13 ± 0.07 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 196 | -0.23 ± 0.09 | None needed (< 0.5 ppm) |
| ^{15}N | 187 | 0.23 ± 0.20 | None needed (< 0.5 ppm) |

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1414 atoms were assigned a chemical shift out of a possible 1547. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone | 632/636 (99%) | 259/261 (99%) | 249/250 (100%) | 124/125 (99%) |
| Sidechain | 782/872 (90%) | 539/578 (93%) | 222/256 (87%) | 21/38 (55%) |
| Aromatic | 0/39 (0%) | 0/19 (0%) | 0/20 (0%) | 0/0 (—%) |
| Overall | 1414/1547 (91%) | 798/858 (93%) | 471/526 (90%) | 145/163 (89%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1995 atoms were assigned a chemical shift out of a possible 2267. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone | 993/1010 (98%) | 412/421 (98%) | 394/398 (99%) | 187/191 (98%) |
| Sidechain | 1002/1151 (87%) | 686/765 (90%) | 295/345 (86%) | 21/41 (51%) |
| Aromatic | 0/106 (0%) | 0/51 (0%) | 0/55 (0%) | 0/0 (—%) |
| Overall | 1995/2267 (88%) | 1098/1237 (89%) | 689/798 (86%) | 208/232 (90%) |

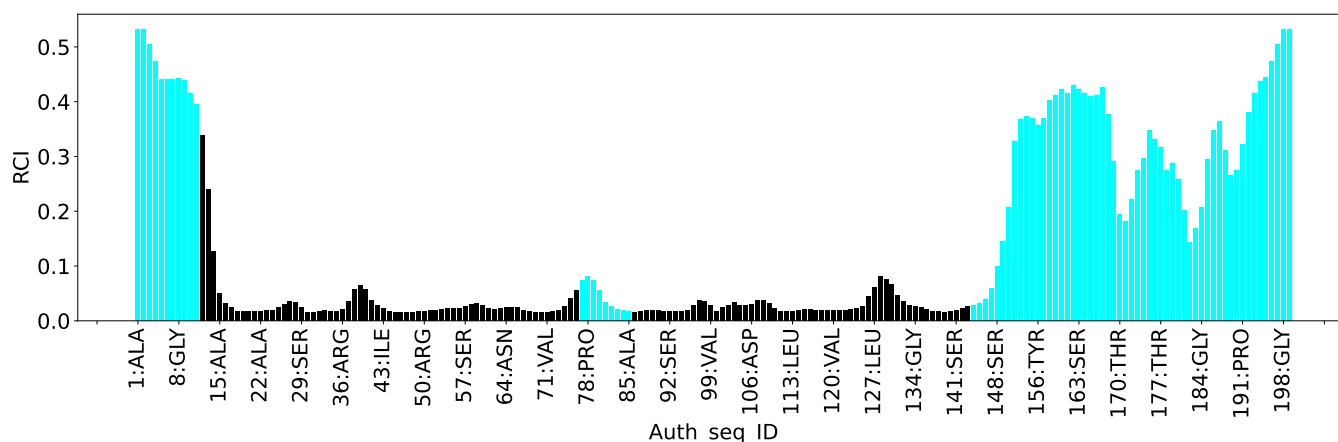
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|--|-------|
| Total distance restraints | 3913 |
| Intra-residue ($ i-j =0$) | 1520 |
| Sequential ($ i-j =1$) | 1068 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 664 |
| Long range ($ i-j \geq 5$) | 661 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 201 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 20.7 |
| 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) | 62.1 | 0.2 |
| 0.2-0.5 (Medium) | 56.4 | 0.5 |
| >0.5 (Large) | 27.2 | 1.99 |

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) | 21.6 | 7.81 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

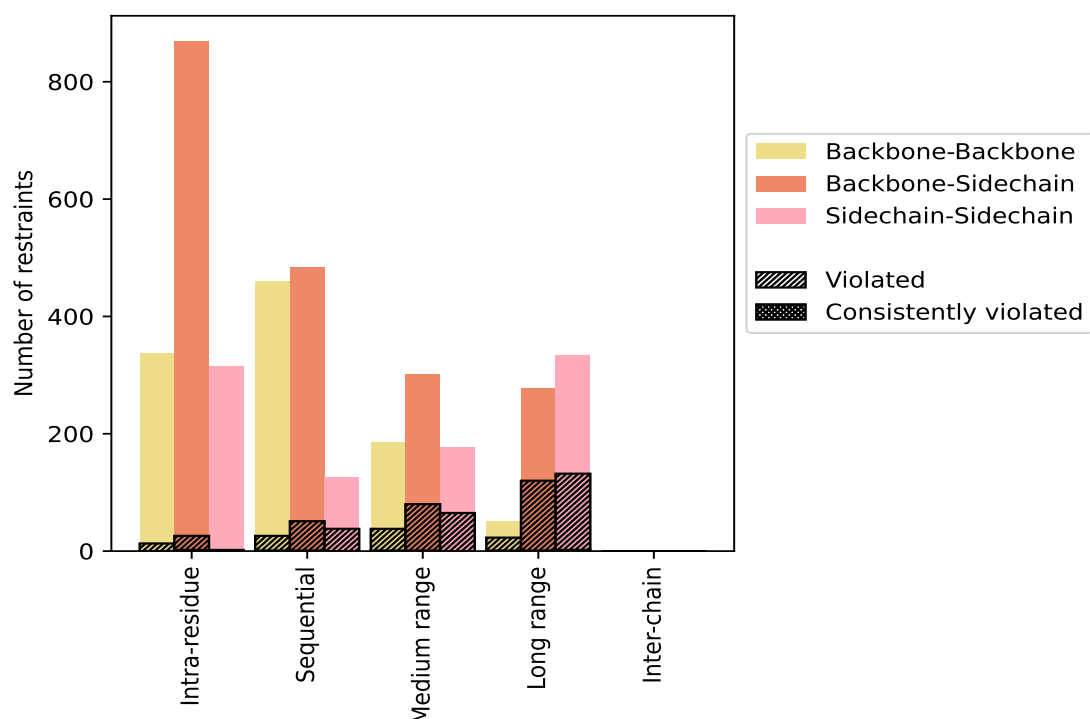
9.1 Summary of distance violations ⓘ

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 ($i-j =0$) | 1520 | 38.8 | 41 | 2.7 | 1.0 | 2 | 0.1 | 0.1 |
| Backbone-Backbone | 337 | 8.6 | 13 | 3.9 | 0.3 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 869 | 22.2 | 26 | 3.0 | 0.7 | 2 | 0.2 | 0.1 |
| Sidechain-Sidechain | 314 | 8.0 | 2 | 0.6 | 0.1 | 0 | 0.0 | 0.0 |
| Sequential ($i-j =1$) | 1068 | 27.3 | 115 | 10.8 | 2.9 | 2 | 0.2 | 0.1 |
| Backbone-Backbone | 460 | 11.8 | 26 | 5.7 | 0.7 | 1 | 0.2 | 0.0 |
| Backbone-Sidechain | 483 | 12.3 | 51 | 10.6 | 1.3 | 1 | 0.2 | 0.0 |
| Sidechain-Sidechain | 125 | 3.2 | 38 | 30.4 | 1.0 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 664 | 17.0 | 183 | 27.6 | 4.7 | 2 | 0.3 | 0.1 |
| Backbone-Backbone | 186 | 4.8 | 38 | 20.4 | 1.0 | 1 | 0.5 | 0.0 |
| Backbone-Sidechain | 302 | 7.7 | 80 | 26.5 | 2.0 | 1 | 0.3 | 0.0 |
| Sidechain-Sidechain | 176 | 4.5 | 65 | 36.9 | 1.7 | 0 | 0.0 | 0.0 |
| Long range ($i-j \geq 5$) | 661 | 16.9 | 275 | 41.6 | 7.0 | 4 | 0.6 | 0.1 |
| Backbone-Backbone | 51 | 1.3 | 23 | 45.1 | 0.6 | 1 | 2.0 | 0.0 |
| Backbone-Sidechain | 277 | 7.1 | 120 | 43.3 | 3.1 | 1 | 0.4 | 0.0 |
| Sidechain-Sidechain | 333 | 8.5 | 132 | 39.6 | 3.4 | 2 | 0.6 | 0.1 |
| Inter-chain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sidechain-Sidechain | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Hydrogen bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 3913 | 100.0 | 614 | 15.7 | 15.7 | 10 | 0.3 | 0.3 |
| Backbone-Backbone | 1034 | 26.4 | 100 | 9.7 | 2.6 | 3 | 0.3 | 0.1 |
| Backbone-Sidechain | 1931 | 49.3 | 277 | 14.3 | 7.1 | 5 | 0.3 | 0.1 |
| Sidechain-Sidechain | 948 | 24.2 | 237 | 25.0 | 6.1 | 2 | 0.2 | 0.1 |

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

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



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

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 9 | 31 | 61 | 49 | 0 | 150 | 0.31 | 1.25 | 0.23 | 0.21 |
| 2 | 11 | 32 | 48 | 51 | 0 | 142 | 0.33 | 1.3 | 0.24 | 0.23 |
| 3 | 8 | 27 | 52 | 66 | 0 | 153 | 0.33 | 1.34 | 0.26 | 0.24 |
| 4 | 13 | 34 | 42 | 59 | 0 | 148 | 0.34 | 1.45 | 0.27 | 0.25 |
| 5 | 14 | 35 | 50 | 62 | 0 | 161 | 0.32 | 1.66 | 0.26 | 0.23 |
| 6 | 14 | 26 | 52 | 73 | 0 | 165 | 0.3 | 1.21 | 0.23 | 0.2 |
| 7 | 12 | 25 | 48 | 53 | 0 | 138 | 0.33 | 1.52 | 0.24 | 0.24 |
| 8 | 9 | 34 | 50 | 55 | 0 | 148 | 0.33 | 1.99 | 0.28 | 0.24 |
| 9 | 14 | 32 | 50 | 67 | 0 | 163 | 0.33 | 1.42 | 0.26 | 0.22 |
| 10 | 13 | 35 | 51 | 77 | 0 | 176 | 0.32 | 1.85 | 0.28 | 0.2 |

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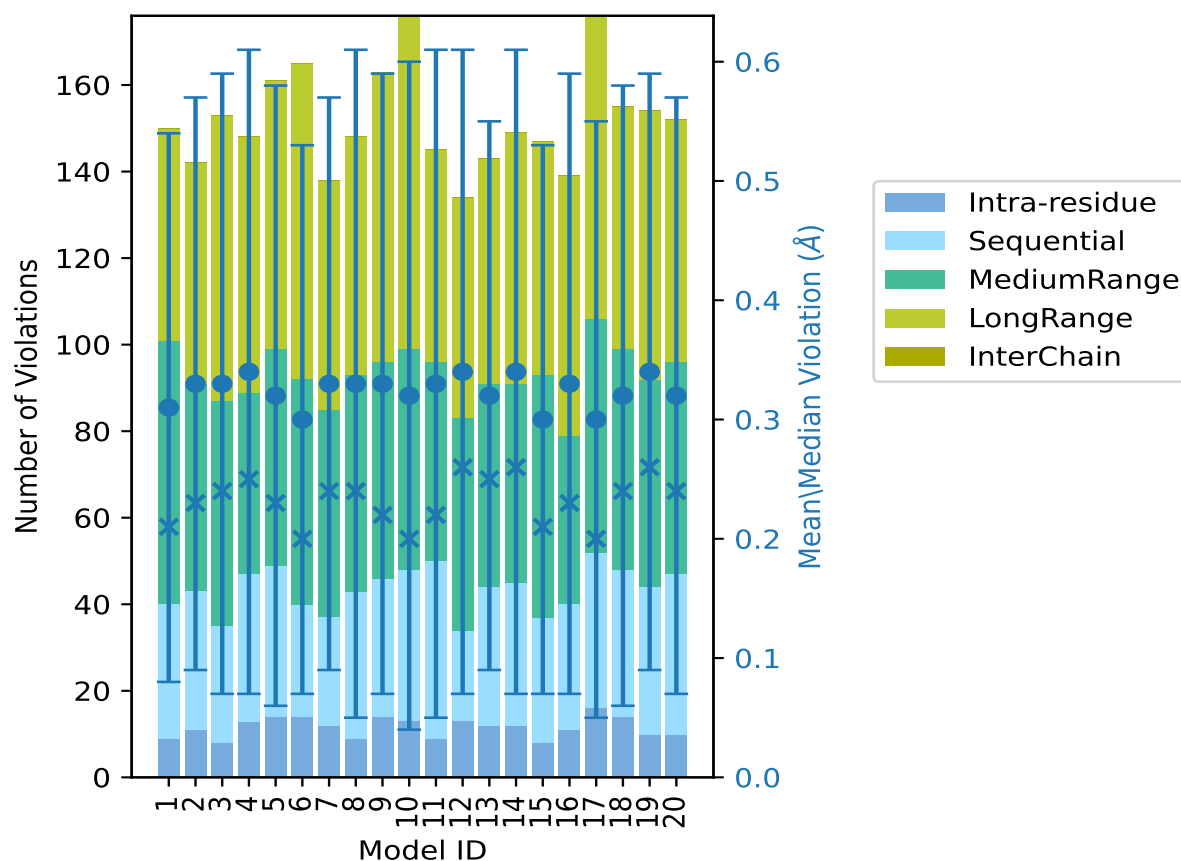
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 9 | 41 | 46 | 49 | 0 | 145 | 0.33 | 1.55 | 0.28 | 0.22 |
| 12 | 13 | 21 | 49 | 51 | 0 | 134 | 0.34 | 1.64 | 0.27 | 0.26 |
| 13 | 12 | 32 | 47 | 52 | 0 | 143 | 0.32 | 1.37 | 0.23 | 0.25 |
| 14 | 12 | 33 | 46 | 58 | 0 | 149 | 0.34 | 1.6 | 0.27 | 0.26 |
| 15 | 8 | 29 | 56 | 54 | 0 | 147 | 0.3 | 1.54 | 0.23 | 0.21 |
| 16 | 11 | 29 | 39 | 60 | 0 | 139 | 0.33 | 1.54 | 0.26 | 0.23 |
| 17 | 16 | 36 | 54 | 70 | 0 | 176 | 0.3 | 1.29 | 0.25 | 0.2 |
| 18 | 14 | 34 | 51 | 56 | 0 | 155 | 0.32 | 1.37 | 0.26 | 0.24 |
| 19 | 10 | 34 | 48 | 62 | 0 | 154 | 0.34 | 1.25 | 0.25 | 0.26 |
| 20 | 10 | 37 | 49 | 56 | 0 | 152 | 0.32 | 1.68 | 0.25 | 0.24 |

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 ⓘ



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

9.3 Distance violation statistics for the ensemble

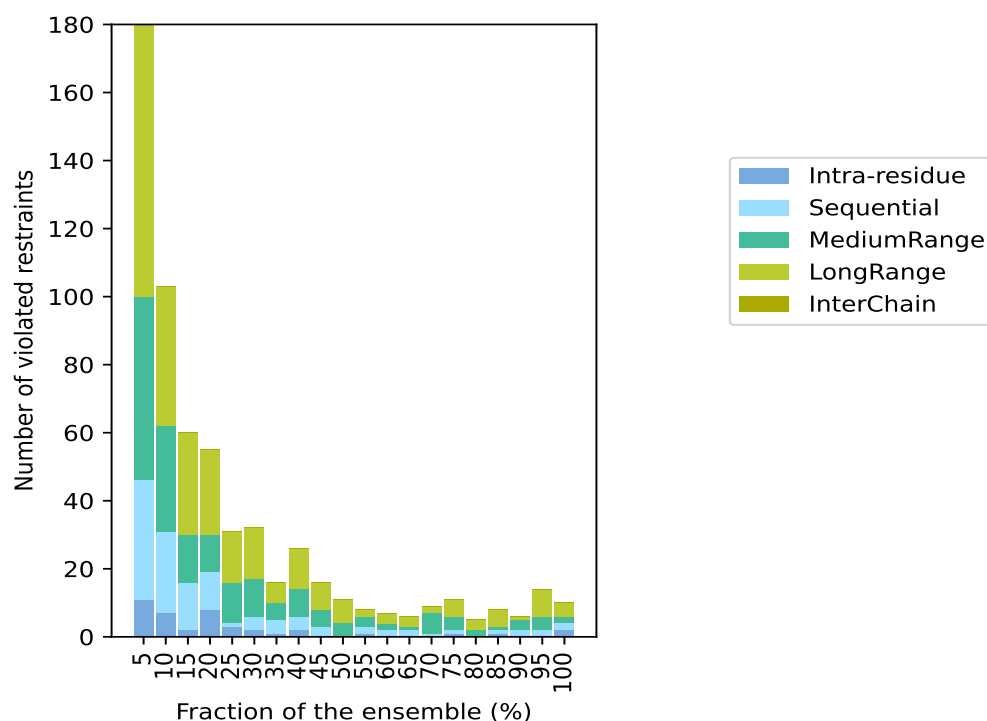
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 3299(IR:1479, SQ:953, MR:481, LR:386, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 11 | 35 | 54 | 80 | 0 | 180 | 1 | 5.0 |
| 7 | 24 | 31 | 41 | 0 | 103 | 2 | 10.0 |
| 2 | 14 | 14 | 30 | 0 | 60 | 3 | 15.0 |
| 8 | 11 | 11 | 25 | 0 | 55 | 4 | 20.0 |
| 3 | 1 | 12 | 15 | 0 | 31 | 5 | 25.0 |
| 2 | 4 | 11 | 15 | 0 | 32 | 6 | 30.0 |
| 1 | 4 | 5 | 6 | 0 | 16 | 7 | 35.0 |
| 2 | 4 | 8 | 12 | 0 | 26 | 8 | 40.0 |
| 0 | 3 | 5 | 8 | 0 | 16 | 9 | 45.0 |
| 0 | 0 | 4 | 7 | 0 | 11 | 10 | 50.0 |
| 1 | 2 | 3 | 2 | 0 | 8 | 11 | 55.0 |
| 0 | 2 | 2 | 3 | 0 | 7 | 12 | 60.0 |
| 0 | 2 | 1 | 3 | 0 | 6 | 13 | 65.0 |
| 0 | 1 | 6 | 2 | 0 | 9 | 14 | 70.0 |
| 1 | 1 | 4 | 5 | 0 | 11 | 15 | 75.0 |
| 0 | 0 | 2 | 3 | 0 | 5 | 16 | 80.0 |
| 1 | 1 | 1 | 5 | 0 | 8 | 17 | 85.0 |
| 0 | 2 | 3 | 1 | 0 | 6 | 18 | 90.0 |
| 0 | 2 | 4 | 8 | 0 | 14 | 19 | 95.0 |
| 2 | 2 | 2 | 4 | 0 | 10 | 20 | 100.0 |

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

⁵Inter-chain restraints, ⁶ Number of models with violations

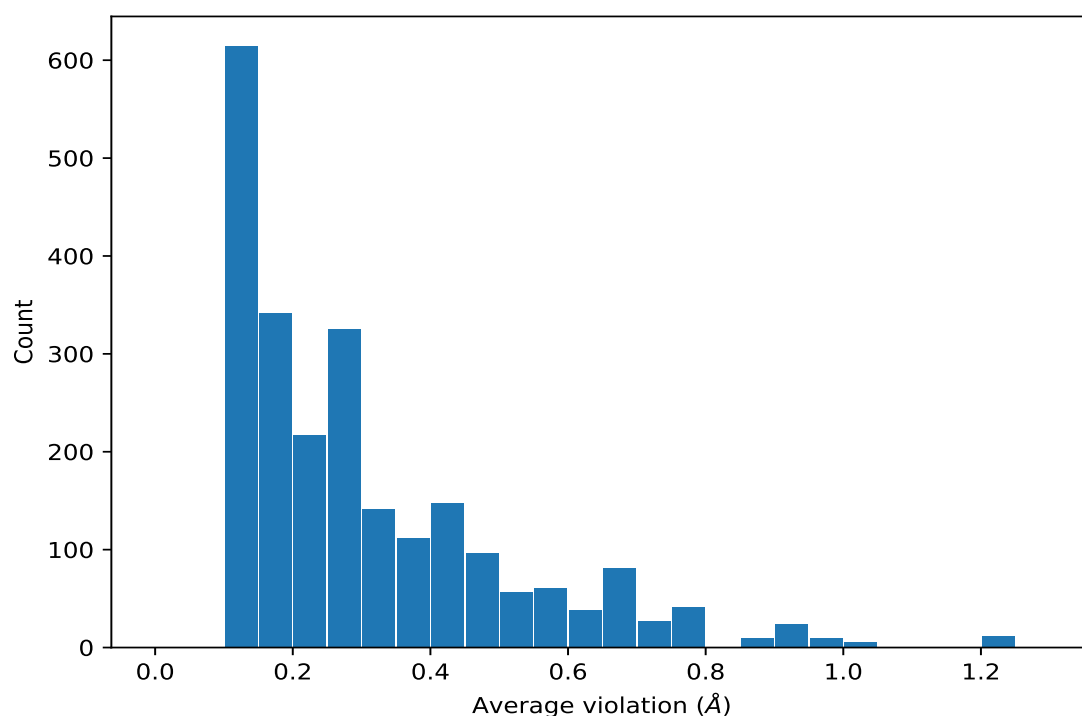
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3553) | 1:87:A:ALA:HB2 | 1:43:A:ILE:HA | 20 | 0.93 | 0.37 | 0.86 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 20 | 0.93 | 0.37 | 0.86 |
| (1,3553) | 1:87:A:ALA:HB3 | 1:43:A:ILE:HA | 20 | 0.93 | 0.37 | 0.86 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:30:A:THR:HB | 20 | 0.93 | 0.37 | 0.86 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD11 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD12 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD13 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD21 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD22 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD23 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD11 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD12 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD13 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD21 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD22 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD23 | 20 | 0.76 | 0.2 | 0.78 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 20 | 0.76 | 0.2 | 0.78 |
| (1,3231) | 1:34:A:VAL:HG22 | 1:139:A:ASP:HA | 20 | 0.71 | 0.21 | 0.77 |
| (1,3231) | 1:34:A:VAL:HG23 | 1:139:A:ASP:HA | 20 | 0.71 | 0.21 | 0.77 |
| (1,3231) | 1:34:A:VAL:HG21 | 1:139:A:ASP:HA | 20 | 0.71 | 0.21 | 0.77 |
| (1,3231) | 1:34:A:VAL:HG13 | 1:36:A:ARG:HA | 20 | 0.71 | 0.21 | 0.77 |
| (1,3231) | 1:34:A:VAL:HG23 | 1:36:A:ARG:HA | 20 | 0.71 | 0.21 | 0.77 |
| (1,3231) | 1:34:A:VAL:HG12 | 1:36:A:ARG:HA | 20 | 0.71 | 0.21 | 0.77 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 20 | 0.54 | 0.13 | 0.54 |
| (1,3353) | 1:11:A:GLY:HA2 | 1:113:A:LEU:HA | 20 | 0.54 | 0.13 | 0.54 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 20 | 0.49 | 0.09 | 0.46 |
| (1,3415) | 1:41:A:GLN:HA | 1:42:A:GLN:HA | 20 | 0.49 | 0.09 | 0.46 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 20 | 0.43 | 0.15 | 0.45 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 20 | 0.43 | 0.15 | 0.45 |
| (1,3464) | 1:126:A:GLY:HA2 | 1:125:A:GLN:HA | 20 | 0.43 | 0.15 | 0.45 |
| (1,3464) | 1:134:A:GLY:HA2 | 1:133:A:SER:HA | 20 | 0.43 | 0.15 | 0.45 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 20 | 0.41 | 0.01 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 20 | 0.41 | 0.01 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 20 | 0.41 | 0.01 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG21 | 20 | 0.41 | 0.01 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG22 | 20 | 0.41 | 0.01 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG23 | 20 | 0.41 | 0.01 | 0.42 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 20 | 0.4 | 0.15 | 0.38 |
| (1,3712) | 1:84:A:SER:HB3 | 1:85:A:ALA:HA | 20 | 0.4 | 0.15 | 0.38 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 20 | 0.27 | 0.08 | 0.29 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 20 | 0.26 | 0.0 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD2 | 1:95:A:PHE:HZ | 20 | 0.26 | 0.0 | 0.26 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB2 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB3 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB2 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB3 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD12 | 1:191:A:PRO:HB2 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD12 | 1:191:A:PRO:HB3 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB2 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB3 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB2 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB3 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB2 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB3 | 19 | 1.22 | 0.4 | 1.32 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA2 | 19 | 0.95 | 0.31 | 1.02 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA3 | 19 | 0.95 | 0.31 | 1.02 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 19 | 0.95 | 0.31 | 1.02 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 19 | 0.95 | 0.31 | 1.02 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA2 | 19 | 0.95 | 0.31 | 1.02 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA3 | 19 | 0.95 | 0.31 | 1.02 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB2 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB3 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB2 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB3 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG11 | 1:117:A:LEU:HB2 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG11 | 1:117:A:LEU:HB3 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB2 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB3 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG23 | 1:117:A:LEU:HB2 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG23 | 1:117:A:LEU:HB3 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG21 | 1:117:A:LEU:HB2 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG21 | 1:117:A:LEU:HB3 | 19 | 0.92 | 0.21 | 0.96 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 19 | 0.69 | 0.34 | 0.65 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD11 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD12 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD13 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD21 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD22 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD23 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD11 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD12 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD13 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD21 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD22 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD23 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD11 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD12 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD13 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD21 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD22 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD23 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD11 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD12 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD13 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD21 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD22 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD23 | 19 | 0.69 | 0.34 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 19 | 0.62 | 0.16 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 19 | 0.62 | 0.16 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 19 | 0.62 | 0.16 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 19 | 0.62 | 0.16 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB2 | 19 | 0.62 | 0.16 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB3 | 19 | 0.62 | 0.16 | 0.65 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 19 | 0.61 | 0.22 | 0.55 |
| (1,3799) | 1:131:A:VAL:HG11 | 1:51:A:ALA:HA | 19 | 0.61 | 0.22 | 0.55 |
| (1,3799) | 1:131:A:VAL:HG13 | 1:51:A:ALA:HA | 19 | 0.61 | 0.22 | 0.55 |
| (1,3799) | 1:131:A:VAL:HG22 | 1:51:A:ALA:HA | 19 | 0.61 | 0.22 | 0.55 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:135:A:SER:HB2 | 19 | 0.61 | 0.22 | 0.55 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:135:A:SER:HB3 | 19 | 0.61 | 0.22 | 0.55 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 19 | 0.59 | 0.14 | 0.63 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 19 | 0.59 | 0.14 | 0.63 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 19 | 0.59 | 0.14 | 0.63 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 19 | 0.59 | 0.14 | 0.63 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 19 | 0.59 | 0.14 | 0.63 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 19 | 0.59 | 0.14 | 0.63 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:14:A:SER:HB2 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:14:A:SER:HB3 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB2 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB3 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA2 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA3 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:14:A:SER:HB2 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:14:A:SER:HB3 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:12:A:GLY:HA2 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:12:A:GLY:HA3 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA2 | 19 | 0.43 | 0.14 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA3 | 19 | 0.43 | 0.14 | 0.35 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 19 | 0.34 | 0.09 | 0.33 |
| (1,1151) | 1:129:A:ILE:H | 1:130:A:ASN:H | 19 | 0.34 | 0.09 | 0.33 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG11 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG11 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG12 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG12 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG13 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG13 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG21 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG21 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG22 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG22 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG23 | 1:95:A:PHE:HE1 | 19 | 0.3 | 0.16 | 0.25 |
| (1,3906) | 1:136:A:VAL:HG23 | 1:95:A:PHE:HE2 | 19 | 0.3 | 0.16 | 0.25 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 19 | 0.28 | 0.07 | 0.26 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 19 | 0.26 | 0.08 | 0.26 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 19 | 0.26 | 0.08 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 19 | 0.23 | 0.07 | 0.23 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 19 | 0.23 | 0.07 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 19 | 0.2 | 0.04 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 19 | 0.2 | 0.04 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 19 | 0.2 | 0.04 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 19 | 0.2 | 0.04 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 19 | 0.2 | 0.04 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 19 | 0.2 | 0.04 | 0.2 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB1 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB2 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB3 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB2 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB3 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:52:A:ALA:HB1 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:52:A:ALA:HB2 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:52:A:ALA:HB3 | 18 | 0.45 | 0.19 | 0.49 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 18 | 0.38 | 0.1 | 0.34 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 18 | 0.38 | 0.1 | 0.34 |
| (1,3798) | 1:164:A:THR:HB | 1:162:A:SER:HA | 18 | 0.38 | 0.1 | 0.34 |
| (1,3798) | 1:161:A:ALA:HA | 1:153:A:SER:HA | 18 | 0.38 | 0.1 | 0.34 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 18 | 0.37 | 0.15 | 0.37 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 18 | 0.37 | 0.15 | 0.37 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB2 | 18 | 0.37 | 0.15 | 0.37 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB3 | 18 | 0.37 | 0.15 | 0.37 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB2 | 18 | 0.37 | 0.15 | 0.37 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB3 | 18 | 0.37 | 0.15 | 0.37 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 18 | 0.29 | 0.08 | 0.29 |
| (1,1107) | 1:109:A:GLY:H | 1:112:A:VAL:HB | 18 | 0.28 | 0.09 | 0.3 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 18 | 0.28 | 0.09 | 0.3 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 18 | 0.28 | 0.1 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 18 | 0.28 | 0.1 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 18 | 0.28 | 0.1 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:123:A:ALA:HB1 | 18 | 0.28 | 0.1 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:123:A:ALA:HB2 | 18 | 0.28 | 0.1 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:123:A:ALA:HB3 | 18 | 0.28 | 0.1 | 0.24 |
| (1,3286) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HB2 | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HB3 | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:47:A:VAL:HB | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB2 | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB3 | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HB2 | 17 | 0.72 | 0.28 | 0.77 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3286) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HB3 | 17 | 0.72 | 0.28 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG21 | 1:47:A:VAL:HB | 17 | 0.72 | 0.28 | 0.77 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 17 | 0.71 | 0.34 | 0.63 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 17 | 0.71 | 0.34 | 0.63 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE1 | 17 | 0.71 | 0.34 | 0.63 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE2 | 17 | 0.71 | 0.34 | 0.63 |
| (1,3623) | 1:140:A:ILE:HD13 | 1:95:A:PHE:HE1 | 17 | 0.71 | 0.34 | 0.63 |
| (1,3623) | 1:140:A:ILE:HD13 | 1:95:A:PHE:HE2 | 17 | 0.71 | 0.34 | 0.63 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD11 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD12 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD13 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD21 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD22 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD23 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG13 | 1:100:A:LEU:HB2 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG13 | 1:100:A:LEU:HB3 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD11 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD12 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD13 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD21 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD22 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD23 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD11 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD12 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD13 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD21 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD22 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD23 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG12 | 1:100:A:LEU:HB2 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG12 | 1:100:A:LEU:HB3 | 17 | 0.69 | 0.4 | 0.51 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 17 | 0.58 | 0.19 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 17 | 0.58 | 0.19 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD11 | 17 | 0.58 | 0.19 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD12 | 17 | 0.58 | 0.19 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD13 | 17 | 0.58 | 0.19 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD21 | 17 | 0.58 | 0.19 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD22 | 17 | 0.58 | 0.19 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD23 | 17 | 0.58 | 0.19 | 0.53 |
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG12 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG13 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB1 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB2 | 17 | 0.49 | 0.23 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB3 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 17 | 0.49 | 0.23 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 17 | 0.49 | 0.23 | 0.52 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB2 | 17 | 0.38 | 0.18 | 0.32 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB3 | 17 | 0.38 | 0.18 | 0.32 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 17 | 0.38 | 0.18 | 0.32 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 17 | 0.38 | 0.18 | 0.32 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 17 | 0.38 | 0.18 | 0.32 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 17 | 0.38 | 0.18 | 0.32 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 17 | 0.37 | 0.15 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 17 | 0.37 | 0.15 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 17 | 0.37 | 0.15 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 17 | 0.37 | 0.15 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 17 | 0.37 | 0.15 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 17 | 0.37 | 0.15 | 0.36 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 17 | 0.13 | 0.01 | 0.13 |
| (1,1132) | 1:59:A:LEU:H | 1:59:A:LEU:HA | 17 | 0.13 | 0.01 | 0.13 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 16 | 0.48 | 0.24 | 0.47 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB2 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB3 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HB2 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HB3 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:132:A:ASP:HB2 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:132:A:ASP:HB3 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:132:A:ASP:HB2 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:132:A:ASP:HB3 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB2 | 16 | 0.44 | 0.22 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB3 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB2 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB3 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HB2 | 16 | 0.44 | 0.22 | 0.38 |
| (1,3422) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HB3 | 16 | 0.44 | 0.22 | 0.38 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:129:A:ILE:HG21 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:129:A:ILE:HG22 | 16 | 0.39 | 0.16 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:129:A:ILE:HG23 | 16 | 0.39 | 0.16 | 0.4 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB1 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB2 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB3 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB1 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB2 | 16 | 0.31 | 0.1 | 0.33 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB3 | 16 | 0.31 | 0.1 | 0.33 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 16 | 0.24 | 0.1 | 0.25 |
| (1,1138) | 1:147:A:LEU:HB2 | 1:149:A:THR:H | 16 | 0.24 | 0.1 | 0.25 |
| (1,1138) | 1:76:A:ARG:HB3 | 1:74:A:VAL:H | 16 | 0.24 | 0.1 | 0.25 |
| (1,1138) | 1:147:A:LEU:HB3 | 1:149:A:THR:H | 16 | 0.24 | 0.1 | 0.25 |
| (1,3849) | 1:51:A:ALA:HB3 | 1:132:A:ASP:HB2 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:51:A:ALA:HB3 | 1:132:A:ASP:HB3 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB2 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB3 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB2 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB3 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB2 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB3 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB2 | 15 | 0.89 | 0.45 | 1.12 |
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB3 | 15 | 0.89 | 0.45 | 1.12 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 15 | 0.76 | 0.35 | 0.82 |
| (1,2430) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HG | 15 | 0.76 | 0.35 | 0.82 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2430) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HG | 15 | 0.76 | 0.35 | 0.82 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:50:A:ARG:HG2 | 15 | 0.76 | 0.35 | 0.82 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:50:A:ARG:HG3 | 15 | 0.76 | 0.35 | 0.82 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD11 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD12 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD13 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD21 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD22 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD23 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD11 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD12 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD13 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD21 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD22 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD23 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG21 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG22 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG23 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG21 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG22 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG23 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD11 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD12 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD13 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD21 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD22 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD23 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HG21 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HG22 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HG23 | 15 | 0.57 | 0.14 | 0.62 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HB2 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HB3 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB2 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB3 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB2 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB3 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB2 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB3 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:10:A:THR:HG23 | 1:42:A:GLN:HB2 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:10:A:THR:HG23 | 1:42:A:GLN:HB3 | 15 | 0.48 | 0.23 | 0.41 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 15 | 0.48 | 0.23 | 0.41 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 15 | 0.48 | 0.16 | 0.5 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 15 | 0.48 | 0.16 | 0.5 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 15 | 0.48 | 0.16 | 0.5 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 15 | 0.48 | 0.16 | 0.5 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 15 | 0.48 | 0.16 | 0.5 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 15 | 0.48 | 0.16 | 0.5 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG11 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG12 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG13 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG21 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG22 | 15 | 0.38 | 0.09 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG23 | 15 | 0.38 | 0.09 | 0.38 |
| (1,3620) | 1:6:A:GLY:HA3 | 1:7:A:PHE:HA | 15 | 0.36 | 0.09 | 0.4 |
| (1,3620) | 1:166:A:GLY:HA2 | 1:163:A:SER:HA | 15 | 0.36 | 0.09 | 0.4 |
| (1,3620) | 1:198:A:GLY:HA2 | 1:197:A:PHE:HA | 15 | 0.36 | 0.09 | 0.4 |
| (1,3620) | 1:193:A:GLY:HA2 | 1:192:A:PHE:HA | 15 | 0.36 | 0.09 | 0.4 |
| (1,3620) | 1:166:A:GLY:HA3 | 1:163:A:SER:HA | 15 | 0.36 | 0.09 | 0.4 |
| (1,3620) | 1:6:A:GLY:HA2 | 1:7:A:PHE:HA | 15 | 0.36 | 0.09 | 0.4 |
| (1,3649) | 1:129:A:ILE:HG21 | 1:131:A:VAL:H | 15 | 0.3 | 0.1 | 0.28 |
| (1,3649) | 1:129:A:ILE:HG22 | 1:131:A:VAL:H | 15 | 0.3 | 0.1 | 0.28 |
| (1,3649) | 1:129:A:ILE:HG23 | 1:131:A:VAL:H | 15 | 0.3 | 0.1 | 0.28 |
| (1,3649) | 1:129:A:ILE:HG22 | 1:129:A:ILE:H | 15 | 0.3 | 0.1 | 0.28 |
| (1,3649) | 1:129:A:ILE:HG23 | 1:129:A:ILE:H | 15 | 0.3 | 0.1 | 0.28 |
| (1,3649) | 1:129:A:ILE:HG21 | 1:129:A:ILE:H | 15 | 0.3 | 0.1 | 0.28 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG11 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG12 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG13 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG21 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG22 | 15 | 0.28 | 0.13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG23 | 15 | 0.28 | 0.13 | 0.27 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 15 | 0.27 | 0.07 | 0.27 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 15 | 0.26 | 0.09 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 15 | 0.26 | 0.09 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 15 | 0.26 | 0.09 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG21 | 15 | 0.26 | 0.09 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG22 | 15 | 0.26 | 0.09 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG23 | 15 | 0.26 | 0.09 | 0.25 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD11 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD12 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD13 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD21 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD22 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD23 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD11 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD12 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD13 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD21 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD22 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD23 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD11 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD12 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD13 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD21 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD22 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD23 | 14 | 0.69 | 0.26 | 0.72 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB1 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB2 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB3 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB1 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB2 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB3 | 14 | 0.53 | 0.26 | 0.57 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 14 | 0.43 | 0.15 | 0.42 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD11 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD12 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD13 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD21 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD22 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD23 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD11 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD12 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD13 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD21 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD22 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD23 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD11 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD12 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD13 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD21 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD22 | 14 | 0.43 | 0.15 | 0.42 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD23 | 14 | 0.43 | 0.15 | 0.42 |
| (1,989) | 1:110:A:SER:H | 1:117:A:LEU:HG | 14 | 0.4 | 0.13 | 0.41 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 14 | 0.4 | 0.13 | 0.41 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 14 | 0.35 | 0.15 | 0.39 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 14 | 0.35 | 0.15 | 0.39 |
| (1,3683) | 1:56:A:ALA:HB1 | 1:50:A:ARG:HA | 14 | 0.31 | 0.16 | 0.27 |
| (1,3683) | 1:56:A:ALA:HB3 | 1:50:A:ARG:HA | 14 | 0.31 | 0.16 | 0.27 |
| (1,3683) | 1:56:A:ALA:HB2 | 1:50:A:ARG:HA | 14 | 0.31 | 0.16 | 0.27 |
| (1,3683) | 1:51:A:ALA:HB1 | 1:50:A:ARG:HA | 14 | 0.31 | 0.16 | 0.27 |
| (1,3683) | 1:51:A:ALA:HB3 | 1:50:A:ARG:HA | 14 | 0.31 | 0.16 | 0.27 |
| (1,3683) | 1:51:A:ALA:HB2 | 1:50:A:ARG:HA | 14 | 0.31 | 0.16 | 0.27 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 14 | 0.23 | 0.09 | 0.21 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 14 | 0.23 | 0.09 | 0.21 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 14 | 0.16 | 0.03 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 14 | 0.16 | 0.03 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 14 | 0.16 | 0.03 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 14 | 0.16 | 0.03 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 14 | 0.16 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 14 | 0.16 | 0.03 | 0.16 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 14 | 0.14 | 0.03 | 0.14 |
| (1,3657) | 1:77:A:LEU:HD23 | 1:73:A:ALA:HA | 13 | 0.73 | 0.39 | 0.7 |
| (1,3657) | 1:77:A:LEU:HD12 | 1:73:A:ALA:HA | 13 | 0.73 | 0.39 | 0.7 |
| (1,3657) | 1:77:A:LEU:HD13 | 1:73:A:ALA:HA | 13 | 0.73 | 0.39 | 0.7 |
| (1,3657) | 1:77:A:LEU:HD22 | 1:73:A:ALA:HA | 13 | 0.73 | 0.39 | 0.7 |
| (1,3657) | 1:77:A:LEU:HD21 | 1:73:A:ALA:HA | 13 | 0.73 | 0.39 | 0.7 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 13 | 0.32 | 0.21 | 0.24 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 13 | 0.32 | 0.21 | 0.24 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 13 | 0.32 | 0.21 | 0.24 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 13 | 0.32 | 0.21 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG2 | 13 | 0.31 | 0.2 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG3 | 13 | 0.31 | 0.2 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG2 | 13 | 0.31 | 0.2 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG3 | 13 | 0.31 | 0.2 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG2 | 13 | 0.31 | 0.2 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG3 | 13 | 0.31 | 0.2 | 0.24 |
| (1,3781) | 1:71:A:VAL:HG12 | 1:68:A:ARG:HG2 | 13 | 0.31 | 0.2 | 0.24 |
| (1,3781) | 1:71:A:VAL:HG12 | 1:68:A:ARG:HG3 | 13 | 0.31 | 0.2 | 0.24 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG11 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG12 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG13 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG21 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG22 | 13 | 0.26 | 0.04 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG23 | 13 | 0.26 | 0.04 | 0.26 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 13 | 0.24 | 0.09 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 13 | 0.24 | 0.09 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 13 | 0.24 | 0.09 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 13 | 0.24 | 0.09 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 13 | 0.24 | 0.09 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 13 | 0.24 | 0.09 | 0.23 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 13 | 0.18 | 0.03 | 0.18 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 13 | 0.18 | 0.03 | 0.18 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 12 | 0.48 | 0.23 | 0.37 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 12 | 0.48 | 0.23 | 0.37 |
| (1,3734) | 1:37:A:THR:HA | 1:136:A:VAL:HB | 12 | 0.48 | 0.23 | 0.37 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3734) | 1:131:A:VAL:HA | 1:136:A:VAL:HB | 12 | 0.48 | 0.23 | 0.37 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB2 | 12 | 0.47 | 0.26 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB3 | 12 | 0.47 | 0.26 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB2 | 12 | 0.47 | 0.26 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB3 | 12 | 0.47 | 0.26 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:157:A:SER:HB2 | 12 | 0.47 | 0.26 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:157:A:SER:HB3 | 12 | 0.47 | 0.26 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:155:A:SER:HB2 | 12 | 0.47 | 0.26 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:155:A:SER:HB3 | 12 | 0.47 | 0.26 | 0.42 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG11 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG12 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG13 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG21 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG22 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG23 | 12 | 0.44 | 0.13 | 0.49 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 12 | 0.42 | 0.21 | 0.38 |
| (1,1031) | 1:170:A:THR:HA | 1:169:A:TYR:H | 12 | 0.42 | 0.21 | 0.38 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 12 | 0.36 | 0.18 | 0.32 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 12 | 0.36 | 0.18 | 0.32 |
| (1,952) | 1:104:A:ASN:HD22 | 1:92:A:SER:HB2 | 12 | 0.36 | 0.18 | 0.32 |
| (1,952) | 1:104:A:ASN:HD22 | 1:92:A:SER:HB3 | 12 | 0.36 | 0.18 | 0.32 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB2 | 12 | 0.32 | 0.14 | 0.35 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB3 | 12 | 0.32 | 0.14 | 0.35 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB2 | 12 | 0.32 | 0.14 | 0.35 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB3 | 12 | 0.32 | 0.14 | 0.35 |
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB2 | 12 | 0.32 | 0.14 | 0.35 |
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB3 | 12 | 0.32 | 0.14 | 0.35 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 12 | 0.17 | 0.02 | 0.18 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 12 | 0.17 | 0.02 | 0.18 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 12 | 0.17 | 0.02 | 0.18 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB1 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB2 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB3 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB1 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB2 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB3 | 11 | 0.64 | 0.31 | 0.67 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3251) | 1:71:A:VAL:HB | 1:51:A:ALA:HB1 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3251) | 1:71:A:VAL:HB | 1:51:A:ALA:HB2 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3251) | 1:71:A:VAL:HB | 1:51:A:ALA:HB3 | 11 | 0.64 | 0.31 | 0.67 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD2 | 11 | 0.46 | 0.26 | 0.42 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD3 | 11 | 0.46 | 0.26 | 0.42 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD2 | 11 | 0.46 | 0.26 | 0.42 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD3 | 11 | 0.46 | 0.26 | 0.42 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD2 | 11 | 0.46 | 0.26 | 0.42 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD3 | 11 | 0.46 | 0.26 | 0.42 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 11 | 0.37 | 0.22 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 11 | 0.37 | 0.22 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 11 | 0.37 | 0.22 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 11 | 0.37 | 0.22 | 0.34 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 11 | 0.32 | 0.15 | 0.32 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 11 | 0.32 | 0.15 | 0.32 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG11 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG12 | 11 | 0.19 | 0.04 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG13 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG21 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG22 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG23 | 11 | 0.19 | 0.04 | 0.19 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 11 | 0.15 | 0.05 | 0.14 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 11 | 0.12 | 0.01 | 0.12 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 11 | 0.11 | 0.0 | 0.11 |
| (1,3793) | 1:48:A:VAL:HG23 | 1:65:A:ASN:HD21 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG23 | 1:65:A:ASN:HD22 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG11 | 1:65:A:ASN:HD21 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG11 | 1:65:A:ASN:HD22 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG13 | 1:65:A:ASN:HD21 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG13 | 1:65:A:ASN:HD22 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD21 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD22 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG22 | 1:65:A:ASN:HD21 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3793) | 1:48:A:VAL:HG22 | 1:65:A:ASN:HD22 | 10 | 0.98 | 0.48 | 1.14 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD11 | 10 | 0.52 | 0.09 | 0.51 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD12 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD13 | 10 | 0.52 | 0.09 | 0.51 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 10 | 0.47 | 0.17 | 0.48 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 10 | 0.47 | 0.17 | 0.48 |
| (1,3759) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB2 | 10 | 0.47 | 0.17 | 0.48 |
| (1,3759) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB3 | 10 | 0.47 | 0.17 | 0.48 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 10 | 0.47 | 0.17 | 0.48 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 10 | 0.47 | 0.17 | 0.48 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD11 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD12 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD13 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD21 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD22 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD23 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 10 | 0.46 | 0.07 | 0.46 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 10 | 0.46 | 0.07 | 0.46 |
| (1,1095) | 1:193:A:GLY:H | 1:191:A:PRO:HA | 10 | 0.37 | 0.19 | 0.34 |
| (1,1095) | 1:193:A:GLY:H | 1:194:A:GLN:HA | 10 | 0.37 | 0.19 | 0.34 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 10 | 0.27 | 0.11 | 0.25 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 10 | 0.26 | 0.15 | 0.18 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 10 | 0.26 | 0.15 | 0.18 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3910) | 1:39:A:VAL:HA | 1:86:A:TYR:HD1 | 10 | 0.26 | 0.15 | 0.18 |
| (1,3910) | 1:39:A:VAL:HA | 1:86:A:TYR:HD2 | 10 | 0.26 | 0.15 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 10 | 0.2 | 0.06 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 10 | 0.2 | 0.06 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG2 | 10 | 0.2 | 0.06 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG3 | 10 | 0.2 | 0.06 | 0.18 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 10 | 0.12 | 0.01 | 0.12 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 10 | 0.11 | 0.01 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 10 | 0.11 | 0.01 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 10 | 0.11 | 0.01 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 10 | 0.11 | 0.01 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 10 | 0.11 | 0.01 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 10 | 0.11 | 0.01 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 10 | 0.11 | 0.01 | 0.11 |
| (1,3632) | 1:44:A:ALA:HB1 | 1:48:A:VAL:HB | 9 | 1.0 | 0.13 | 1.03 |
| (1,3632) | 1:44:A:ALA:HB2 | 1:48:A:VAL:HB | 9 | 1.0 | 0.13 | 1.03 |
| (1,3632) | 1:44:A:ALA:HB2 | 1:43:A:ILE:HB | 9 | 1.0 | 0.13 | 1.03 |
| (1,3632) | 1:44:A:ALA:HB3 | 1:43:A:ILE:HB | 9 | 1.0 | 0.13 | 1.03 |
| (1,3632) | 1:44:A:ALA:HB3 | 1:48:A:VAL:HB | 9 | 1.0 | 0.13 | 1.03 |
| (1,3632) | 1:44:A:ALA:HB1 | 1:43:A:ILE:HB | 9 | 1.0 | 0.13 | 1.03 |
| (1,3790) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 9 | 0.49 | 0.24 | 0.47 |
| (1,3790) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 9 | 0.49 | 0.24 | 0.47 |
| (1,3790) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HA | 9 | 0.49 | 0.24 | 0.47 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 9 | 0.37 | 0.2 | 0.25 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 9 | 0.37 | 0.2 | 0.25 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 9 | 0.32 | 0.16 | 0.3 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 9 | 0.32 | 0.16 | 0.3 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB2 | 9 | 0.32 | 0.16 | 0.3 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB3 | 9 | 0.32 | 0.16 | 0.3 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD11 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD12 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD13 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD21 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD22 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD23 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD11 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD12 | 9 | 0.3 | 0.08 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD13 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD21 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD22 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD23 | 9 | 0.3 | 0.08 | 0.32 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 9 | 0.29 | 0.07 | 0.29 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 9 | 0.29 | 0.07 | 0.29 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 9 | 0.29 | 0.07 | 0.29 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD11 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD12 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD13 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD21 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD22 | 9 | 0.27 | 0.08 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD23 | 9 | 0.27 | 0.08 | 0.3 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG11 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG12 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG13 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG21 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG22 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG23 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 9 | 0.27 | 0.1 | 0.21 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 9 | 0.23 | 0.07 | 0.25 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 9 | 0.23 | 0.07 | 0.25 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 9 | 0.23 | 0.09 | 0.2 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 9 | 0.23 | 0.09 | 0.2 |
| (1,3334) | 1:25:A:LEU:HA | 1:190:A:ALA:HA | 9 | 0.23 | 0.09 | 0.2 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 9 | 0.23 | 0.08 | 0.25 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 9 | 0.23 | 0.08 | 0.25 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 9 | 0.21 | 0.1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 9 | 0.21 | 0.1 | 0.17 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 9 | 0.2 | 0.07 | 0.18 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 9 | 0.2 | 0.07 | 0.18 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 9 | 0.18 | 0.07 | 0.16 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 9 | 0.18 | 0.07 | 0.16 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 9 | 0.18 | 0.07 | 0.16 |
| (1,949) | 1:55:A:LEU:H | 1:129:A:ILE:HD11 | 9 | 0.18 | 0.07 | 0.16 |
| (1,949) | 1:55:A:LEU:H | 1:129:A:ILE:HD12 | 9 | 0.18 | 0.07 | 0.16 |
| (1,949) | 1:55:A:LEU:H | 1:129:A:ILE:HD13 | 9 | 0.18 | 0.07 | 0.16 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 9 | 0.16 | 0.04 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 9 | 0.16 | 0.04 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 9 | 0.16 | 0.04 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 9 | 0.16 | 0.04 | 0.14 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 9 | 0.12 | 0.02 | 0.12 |
| (1,3292) | 1:112:A:VAL:H | 1:108:A:LEU:HG | 8 | 0.56 | 0.15 | 0.55 |
| (1,3292) | 1:13:A:ALA:H | 1:108:A:LEU:HG | 8 | 0.56 | 0.15 | 0.55 |
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 8 | 0.47 | 0.15 | 0.41 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG2 | 8 | 0.44 | 0.25 | 0.4 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG3 | 8 | 0.44 | 0.25 | 0.4 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG2 | 8 | 0.44 | 0.25 | 0.4 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG3 | 8 | 0.44 | 0.25 | 0.4 |
| (1,3735) | 1:48:A:VAL:HG22 | 1:46:A:SER:H | 8 | 0.43 | 0.24 | 0.38 |
| (1,3735) | 1:48:A:VAL:HG23 | 1:46:A:SER:H | 8 | 0.43 | 0.24 | 0.38 |
| (1,3735) | 1:48:A:VAL:HG21 | 1:46:A:SER:H | 8 | 0.43 | 0.24 | 0.38 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA2 | 8 | 0.4 | 0.11 | 0.39 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA3 | 8 | 0.4 | 0.11 | 0.39 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA2 | 8 | 0.4 | 0.11 | 0.39 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA3 | 8 | 0.4 | 0.11 | 0.39 |
| (1,3238) | 1:129:A:ILE:HD13 | 1:128:A:GLY:HA2 | 8 | 0.4 | 0.11 | 0.39 |
| (1,3238) | 1:129:A:ILE:HD13 | 1:128:A:GLY:HA3 | 8 | 0.4 | 0.11 | 0.39 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG11 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG12 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG13 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG21 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG22 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG23 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG11 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG12 | 8 | 0.38 | 0.11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG13 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG21 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG22 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG23 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG11 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG12 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG13 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG21 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG22 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG23 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG11 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG12 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG13 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG21 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG22 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG23 | 8 | 0.38 | 0.11 | 0.36 |
| (1,3419) | 1:18:A:ILE:HG12 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:18:A:ILE:HG12 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:18:A:ILE:HG13 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:18:A:ILE:HG13 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG2 | 8 | 0.35 | 0.14 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG3 | 8 | 0.35 | 0.14 | 0.32 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 8 | 0.27 | 0.18 | 0.21 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 8 | 0.27 | 0.18 | 0.21 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 8 | 0.27 | 0.09 | 0.26 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 8 | 0.27 | 0.09 | 0.26 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 8 | 0.27 | 0.09 | 0.26 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 8 | 0.27 | 0.09 | 0.26 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 8 | 0.27 | 0.12 | 0.22 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 8 | 0.27 | 0.12 | 0.22 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB2 | 8 | 0.25 | 0.1 | 0.24 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB3 | 8 | 0.25 | 0.1 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1148) | 1:134:A:GLY:H | 1:67:A:ALA:HA | 8 | 0.25 | 0.1 | 0.24 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB2 | 8 | 0.24 | 0.09 | 0.26 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB3 | 8 | 0.24 | 0.09 | 0.26 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB2 | 8 | 0.24 | 0.09 | 0.26 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB3 | 8 | 0.24 | 0.09 | 0.26 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 8 | 0.23 | 0.14 | 0.18 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD11 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD12 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD13 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD21 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD22 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD23 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD11 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD12 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD13 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD21 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD22 | 8 | 0.2 | 0.05 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD23 | 8 | 0.2 | 0.05 | 0.2 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 8 | 0.2 | 0.1 | 0.16 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 8 | 0.2 | 0.1 | 0.16 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 8 | 0.18 | 0.04 | 0.16 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 8 | 0.18 | 0.04 | 0.16 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 8 | 0.17 | 0.05 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 8 | 0.17 | 0.04 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 8 | 0.17 | 0.04 | 0.18 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 8 | 0.16 | 0.04 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 8 | 0.16 | 0.04 | 0.16 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 8 | 0.16 | 0.06 | 0.14 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 8 | 0.16 | 0.06 | 0.14 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 8 | 0.16 | 0.06 | 0.14 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 8 | 0.16 | 0.06 | 0.14 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 8 | 0.16 | 0.03 | 0.16 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 8 | 0.16 | 0.03 | 0.16 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 8 | 0.14 | 0.03 | 0.14 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 8 | 0.14 | 0.03 | 0.14 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 8 | 0.12 | 0.01 | 0.12 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 8 | 0.12 | 0.01 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 8 | 0.12 | 0.01 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 8 | 0.12 | 0.01 | 0.12 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB1 | 7 | 0.56 | 0.11 | 0.6 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB2 | 7 | 0.56 | 0.11 | 0.6 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB3 | 7 | 0.56 | 0.11 | 0.6 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB1 | 7 | 0.56 | 0.11 | 0.6 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB2 | 7 | 0.56 | 0.11 | 0.6 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB3 | 7 | 0.56 | 0.11 | 0.6 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD11 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD12 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD13 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:129:A:ILE:HD11 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:129:A:ILE:HD12 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:129:A:ILE:HD13 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD11 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD12 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD13 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD21 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD22 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD23 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB1 | 1:129:A:ILE:HD11 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB1 | 1:129:A:ILE:HD12 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB1 | 1:129:A:ILE:HD13 | 7 | 0.42 | 0.12 | 0.36 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 7 | 0.29 | 0.15 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 7 | 0.29 | 0.15 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 7 | 0.29 | 0.15 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 7 | 0.29 | 0.15 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 7 | 0.29 | 0.15 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 7 | 0.29 | 0.15 | 0.31 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 7 | 0.28 | 0.09 | 0.28 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 7 | 0.28 | 0.09 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB1 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB2 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB3 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB1 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB2 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB3 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG23 | 1:73:A:ALA:HB1 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG23 | 1:73:A:ALA:HB2 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG23 | 1:73:A:ALA:HB3 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB1 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB2 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB3 | 7 | 0.24 | 0.05 | 0.26 |
| (1,3796) | 1:124:A:ALA:HB2 | 1:120:A:VAL:HA | 7 | 0.23 | 0.12 | 0.19 |
| (1,3796) | 1:124:A:ALA:HB3 | 1:120:A:VAL:HA | 7 | 0.23 | 0.12 | 0.19 |
| (1,3796) | 1:124:A:ALA:HB1 | 1:120:A:VAL:HA | 7 | 0.23 | 0.12 | 0.19 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 7 | 0.2 | 0.05 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 7 | 0.2 | 0.05 | 0.17 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 7 | 0.18 | 0.05 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 7 | 0.17 | 0.05 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 7 | 0.17 | 0.05 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 7 | 0.17 | 0.05 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 7 | 0.17 | 0.05 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 7 | 0.17 | 0.05 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 7 | 0.17 | 0.05 | 0.15 |
| (1,3515) | 1:31:A:LEU:HD23 | 1:31:A:LEU:HA | 7 | 0.16 | 0.03 | 0.17 |
| (1,3515) | 1:31:A:LEU:HD22 | 1:31:A:LEU:HA | 7 | 0.16 | 0.03 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3515) | 1:31:A:LEU:HD21 | 1:31:A:LEU:HA | 7 | 0.16 | 0.03 | 0.17 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 7 | 0.16 | 0.04 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 7 | 0.16 | 0.04 | 0.16 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 7 | 0.15 | 0.04 | 0.14 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 7 | 0.15 | 0.04 | 0.14 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 7 | 0.15 | 0.03 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 7 | 0.15 | 0.03 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 7 | 0.15 | 0.03 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 7 | 0.15 | 0.03 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 7 | 0.15 | 0.03 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 7 | 0.15 | 0.03 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 7 | 0.14 | 0.02 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 7 | 0.14 | 0.02 | 0.15 |
| (1,1156) | 1:34:A:VAL:H | 1:34:A:VAL:HA | 7 | 0.12 | 0.01 | 0.12 |
| (1,1156) | 1:31:A:LEU:H | 1:31:A:LEU:HA | 7 | 0.12 | 0.01 | 0.12 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB1 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB2 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB3 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:159:A:ALA:HB1 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:159:A:ALA:HB2 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:159:A:ALA:HB3 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB3 | 1:161:A:ALA:HB1 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB3 | 1:161:A:ALA:HB2 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB3 | 1:161:A:ALA:HB3 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:3:A:PRO:HB3 | 1:9:A:ALA:HB1 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:3:A:PRO:HB3 | 1:9:A:ALA:HB2 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3785) | 1:3:A:PRO:HB3 | 1:9:A:ALA:HB3 | 6 | 0.6 | 0.27 | 0.58 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB2 | 6 | 0.41 | 0.26 | 0.3 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB3 | 6 | 0.41 | 0.26 | 0.3 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:46:A:SER:HB2 | 6 | 0.41 | 0.26 | 0.3 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:46:A:SER:HB3 | 6 | 0.41 | 0.26 | 0.3 |
| (1,3763) | 1:41:A:GLN:HB3 | 1:45:A:SER:HB2 | 6 | 0.41 | 0.26 | 0.3 |
| (1,3763) | 1:41:A:GLN:HB3 | 1:45:A:SER:HB3 | 6 | 0.41 | 0.26 | 0.3 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD11 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD12 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD13 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD21 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD22 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD23 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3660) | 1:172:A:PRO:HG2 | 1:18:A:ILE:HG12 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3660) | 1:172:A:PRO:HG2 | 1:18:A:ILE:HG13 | 6 | 0.38 | 0.2 | 0.36 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB1 | 6 | 0.36 | 0.14 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB2 | 6 | 0.36 | 0.14 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB3 | 6 | 0.36 | 0.14 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB1 | 6 | 0.36 | 0.14 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB2 | 6 | 0.36 | 0.14 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB3 | 6 | 0.36 | 0.14 | 0.34 |
| (1,1065) | 1:50:A:ARG:HB2 | 1:50:A:ARG:HE | 6 | 0.35 | 0.14 | 0.32 |
| (1,1065) | 1:50:A:ARG:HB3 | 1:50:A:ARG:HE | 6 | 0.35 | 0.14 | 0.32 |
| (1,1065) | 1:111:A:ARG:HB2 | 1:111:A:ARG:HE | 6 | 0.35 | 0.14 | 0.32 |
| (1,3268) | 1:9:A:ALA:HA | 1:113:A:LEU:HG | 6 | 0.3 | 0.12 | 0.28 |
| (1,3268) | 1:10:A:THR:HA | 1:113:A:LEU:HG | 6 | 0.3 | 0.12 | 0.28 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE21 | 6 | 0.3 | 0.13 | 0.26 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE22 | 6 | 0.3 | 0.13 | 0.26 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE21 | 6 | 0.3 | 0.13 | 0.26 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE22 | 6 | 0.3 | 0.13 | 0.26 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD11 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD12 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD13 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD21 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD22 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD23 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD11 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD12 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD13 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD21 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD22 | 6 | 0.26 | 0.13 | 0.26 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD23 | 6 | 0.26 | 0.13 | 0.26 |
| (1,1803) | 1:177:A:THR:H | 1:175:A:PRO:HA | 6 | 0.24 | 0.21 | 0.16 |
| (1,1803) | 1:177:A:THR:H | 1:179:A:PRO:HA | 6 | 0.24 | 0.21 | 0.16 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB2 | 6 | 0.23 | 0.07 | 0.24 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB3 | 6 | 0.23 | 0.07 | 0.24 |
| (1,1123) | 1:132:A:ASP:H | 1:136:A:VAL:HB | 6 | 0.22 | 0.1 | 0.18 |
| (1,1123) | 1:132:A:ASP:H | 1:71:A:VAL:HB | 6 | 0.22 | 0.1 | 0.18 |
| (1,3844) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 6 | 0.2 | 0.04 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD11 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD12 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD13 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD21 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD22 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD23 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG11 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG12 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG13 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG21 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG22 | 6 | 0.19 | 0.05 | 0.2 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG23 | 6 | 0.19 | 0.05 | 0.2 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD11 | 6 | 0.19 | 0.07 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD12 | 6 | 0.19 | 0.07 | 0.16 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD13 | 6 | 0.19 | 0.07 | 0.16 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD21 | 6 | 0.19 | 0.07 | 0.16 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD22 | 6 | 0.19 | 0.07 | 0.16 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD23 | 6 | 0.19 | 0.07 | 0.16 |
| (1,1904) | 1:20:A:ARG:HA | 1:24:A:ALA:HA | 6 | 0.18 | 0.1 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE1 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE2 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE1 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE2 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE1 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE2 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE1 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE2 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE1 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE2 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE1 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE2 | 6 | 0.18 | 0.11 | 0.15 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB2 | 6 | 0.17 | 0.05 | 0.16 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB3 | 6 | 0.17 | 0.05 | 0.16 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB2 | 6 | 0.17 | 0.05 | 0.16 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB3 | 6 | 0.17 | 0.05 | 0.16 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG21 | 6 | 0.17 | 0.03 | 0.18 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG22 | 6 | 0.17 | 0.03 | 0.18 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG23 | 6 | 0.17 | 0.03 | 0.18 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD21 | 6 | 0.16 | 0.06 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD22 | 6 | 0.16 | 0.06 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD21 | 6 | 0.16 | 0.06 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD22 | 6 | 0.16 | 0.06 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD1 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD2 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD1 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD2 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD1 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD2 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG21 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG22 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG23 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG21 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG22 | 6 | 0.16 | 0.03 | 0.16 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG23 | 6 | 0.16 | 0.03 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB2 | 6 | 0.15 | 0.04 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB3 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB2 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB3 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB2 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB3 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB2 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB3 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB2 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB3 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB2 | 6 | 0.15 | 0.04 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB3 | 6 | 0.15 | 0.04 | 0.16 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB2 | 6 | 0.15 | 0.02 | 0.15 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB3 | 6 | 0.15 | 0.02 | 0.15 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG21 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG22 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG23 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG21 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG22 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG23 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG21 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG22 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG23 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG21 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG22 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG23 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG21 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG22 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG23 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG21 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG22 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG23 | 6 | 0.14 | 0.04 | 0.14 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 6 | 0.14 | 0.03 | 0.13 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 6 | 0.14 | 0.03 | 0.13 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 6 | 0.14 | 0.03 | 0.13 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 6 | 0.14 | 0.03 | 0.13 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 6 | 0.14 | 0.03 | 0.13 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 6 | 0.14 | 0.03 | 0.13 |
| (1,455) | 1:83:A:THR:HG21 | 1:84:A:SER:H | 6 | 0.13 | 0.02 | 0.14 |
| (1,455) | 1:83:A:THR:HG22 | 1:84:A:SER:H | 6 | 0.13 | 0.02 | 0.14 |
| (1,455) | 1:83:A:THR:HG23 | 1:84:A:SER:H | 6 | 0.13 | 0.02 | 0.14 |
| (1,3005) | 1:37:A:THR:HG21 | 1:136:A:VAL:HA | 6 | 0.13 | 0.03 | 0.14 |
| (1,3005) | 1:37:A:THR:HG22 | 1:136:A:VAL:HA | 6 | 0.13 | 0.03 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3005) | 1:37:A:THR:HG23 | 1:136:A:VAL:HA | 6 | 0.13 | 0.03 | 0.14 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG2 | 6 | 0.13 | 0.02 | 0.12 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG3 | 6 | 0.13 | 0.02 | 0.12 |
| (1,1707) | 1:149:A:THR:H | 1:149:A:THR:HA | 6 | 0.12 | 0.0 | 0.12 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB2 | 6 | 0.12 | 0.01 | 0.12 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB3 | 6 | 0.12 | 0.01 | 0.12 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD11 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD12 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD13 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:105:A:ILE:HD11 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:105:A:ILE:HD12 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:105:A:ILE:HD13 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB1 | 1:105:A:ILE:HD11 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB1 | 1:105:A:ILE:HD12 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB1 | 1:105:A:ILE:HD13 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG11 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG12 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG13 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG21 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG22 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG23 | 5 | 0.61 | 0.22 | 0.71 |
| (1,3791) | 1:44:A:ALA:HB1 | 1:74:A:VAL:HA | 5 | 0.47 | 0.23 | 0.49 |
| (1,3791) | 1:44:A:ALA:HB2 | 1:74:A:VAL:HA | 5 | 0.47 | 0.23 | 0.49 |
| (1,3791) | 1:44:A:ALA:HB3 | 1:74:A:VAL:HA | 5 | 0.47 | 0.23 | 0.49 |
| (1,3695) | 1:150:A:SER:HB3 | 1:147:A:LEU:HA | 5 | 0.35 | 0.14 | 0.42 |
| (1,3695) | 1:195:A:SER:HB2 | 1:102:A:ALA:HA | 5 | 0.35 | 0.14 | 0.42 |
| (1,3695) | 1:150:A:SER:HB2 | 1:147:A:LEU:HA | 5 | 0.35 | 0.14 | 0.42 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB2 | 5 | 0.34 | 0.07 | 0.35 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB3 | 5 | 0.34 | 0.07 | 0.35 |
| (1,3473) | 1:21:A:VAL:HG11 | 1:92:A:SER:HA | 5 | 0.33 | 0.1 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG12 | 1:92:A:SER:HA | 5 | 0.33 | 0.1 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG13 | 1:92:A:SER:HA | 5 | 0.33 | 0.1 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG21 | 1:92:A:SER:HA | 5 | 0.33 | 0.1 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG22 | 1:92:A:SER:HA | 5 | 0.33 | 0.1 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG23 | 1:92:A:SER:HA | 5 | 0.33 | 0.1 | 0.37 |
| (1,3655) | 1:87:A:ALA:HB1 | 1:35:A:LEU:HA | 5 | 0.31 | 0.16 | 0.25 |
| (1,3655) | 1:87:A:ALA:HB3 | 1:39:A:VAL:HA | 5 | 0.31 | 0.16 | 0.25 |
| (1,3655) | 1:87:A:ALA:HB2 | 1:35:A:LEU:HA | 5 | 0.31 | 0.16 | 0.25 |
| (1,3655) | 1:87:A:ALA:HB2 | 1:39:A:VAL:HA | 5 | 0.31 | 0.16 | 0.25 |
| (1,3655) | 1:87:A:ALA:HB3 | 1:35:A:LEU:HA | 5 | 0.31 | 0.16 | 0.25 |
| (1,3654) | 1:39:A:VAL:HG13 | 1:38:A:GLY:HA2 | 5 | 0.31 | 0.16 | 0.22 |
| (1,3654) | 1:39:A:VAL:HG13 | 1:38:A:GLY:HA3 | 5 | 0.31 | 0.16 | 0.22 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3654) | 1:39:A:VAL:HG12 | 1:38:A:GLY:HA2 | 5 | 0.31 | 0.16 | 0.22 |
| (1,3654) | 1:39:A:VAL:HG12 | 1:38:A:GLY:HA3 | 5 | 0.31 | 0.16 | 0.22 |
| (1,3654) | 1:39:A:VAL:HG11 | 1:38:A:GLY:HA2 | 5 | 0.31 | 0.16 | 0.22 |
| (1,3654) | 1:39:A:VAL:HG11 | 1:38:A:GLY:HA3 | 5 | 0.31 | 0.16 | 0.22 |
| (1,3545) | 1:55:A:LEU:HD21 | 1:49:A:GLN:HB2 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD21 | 1:49:A:GLN:HB3 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD22 | 1:49:A:GLN:HB2 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD22 | 1:49:A:GLN:HB3 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD23 | 1:49:A:GLN:HB2 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD23 | 1:49:A:GLN:HB3 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD13 | 1:49:A:GLN:HB2 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD13 | 1:49:A:GLN:HB3 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 5 | 0.3 | 0.32 | 0.15 |
| (1,3545) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 5 | 0.3 | 0.32 | 0.15 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD21 | 5 | 0.28 | 0.02 | 0.29 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD22 | 5 | 0.28 | 0.02 | 0.29 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB2 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB3 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB2 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB3 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HB2 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HB3 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HB2 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HB3 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HB2 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3474) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HB3 | 5 | 0.24 | 0.09 | 0.24 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD11 | 5 | 0.22 | 0.12 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD12 | 5 | 0.22 | 0.12 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD13 | 5 | 0.22 | 0.12 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD21 | 5 | 0.22 | 0.12 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD22 | 5 | 0.22 | 0.12 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD23 | 5 | 0.22 | 0.12 | 0.15 |
| (1,781) | 1:127:A:LEU:H | 1:129:A:ILE:H | 5 | 0.19 | 0.06 | 0.16 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG21 | 5 | 0.19 | 0.05 | 0.19 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG22 | 5 | 0.19 | 0.05 | 0.19 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG23 | 5 | 0.19 | 0.05 | 0.19 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD11 | 5 | 0.18 | 0.05 | 0.17 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD12 | 5 | 0.18 | 0.05 | 0.17 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD13 | 5 | 0.18 | 0.05 | 0.17 |
| (1,2112) | 1:41:A:GLN:HE21 | 1:45:A:SER:HA | 5 | 0.18 | 0.06 | 0.2 |
| (1,2112) | 1:41:A:GLN:HE22 | 1:45:A:SER:HA | 5 | 0.18 | 0.06 | 0.2 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA2 | 5 | 0.18 | 0.04 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA3 | 5 | 0.18 | 0.04 | 0.16 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA2 | 5 | 0.17 | 0.04 | 0.17 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA3 | 5 | 0.17 | 0.04 | 0.17 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD21 | 5 | 0.16 | 0.03 | 0.15 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD22 | 5 | 0.16 | 0.03 | 0.15 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA2 | 5 | 0.15 | 0.04 | 0.16 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA3 | 5 | 0.15 | 0.04 | 0.16 |
| (1,2609) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HA | 5 | 0.15 | 0.02 | 0.15 |
| (1,2609) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HA | 5 | 0.15 | 0.02 | 0.15 |
| (1,728) | 1:116:A:LEU:H | 1:120:A:VAL:H | 5 | 0.14 | 0.04 | 0.13 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB2 | 5 | 0.14 | 0.02 | 0.13 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB3 | 5 | 0.14 | 0.02 | 0.13 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE1 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE1 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE1 | 5 | 0.14 | 0.02 | 0.14 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,295) | 1:50:A:ARG:HB2 | 1:57:A:SER:H | 5 | 0.14 | 0.04 | 0.13 |
| (1,295) | 1:50:A:ARG:HB3 | 1:57:A:SER:H | 5 | 0.14 | 0.04 | 0.13 |
| (1,589) | 1:101:A:ASN:H | 1:104:A:ASN:H | 5 | 0.14 | 0.02 | 0.12 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG21 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG22 | 5 | 0.14 | 0.02 | 0.14 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG23 | 5 | 0.14 | 0.02 | 0.14 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB2 | 5 | 0.14 | 0.02 | 0.14 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB3 | 5 | 0.14 | 0.02 | 0.14 |
| (1,2280) | 1:62:A:ASP:HA | 1:66:A:LEU:HG | 5 | 0.13 | 0.03 | 0.12 |
| (1,3021) | 1:28:A:THR:HG21 | 1:139:A:ASP:HA | 5 | 0.13 | 0.02 | 0.13 |
| (1,3021) | 1:28:A:THR:HG22 | 1:139:A:ASP:HA | 5 | 0.13 | 0.02 | 0.13 |
| (1,3021) | 1:28:A:THR:HG23 | 1:139:A:ASP:HA | 5 | 0.13 | 0.02 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG11 | 5 | 0.12 | 0.01 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG12 | 5 | 0.12 | 0.01 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG13 | 5 | 0.12 | 0.01 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG21 | 5 | 0.12 | 0.01 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG22 | 5 | 0.12 | 0.01 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG23 | 5 | 0.12 | 0.01 | 0.13 |
| (1,3711) | 1:149:A:THR:H | 1:149:A:THR:HA | 5 | 0.12 | 0.0 | 0.12 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB1 | 4 | 0.66 | 0.24 | 0.55 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB2 | 4 | 0.66 | 0.24 | 0.55 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB3 | 4 | 0.66 | 0.24 | 0.55 |
| (1,3768) | 1:172:A:PRO:HG2 | 1:24:A:ALA:HB1 | 4 | 0.66 | 0.24 | 0.55 |
| (1,3768) | 1:172:A:PRO:HG2 | 1:24:A:ALA:HB2 | 4 | 0.66 | 0.24 | 0.55 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3768) | 1:172:A:PRO:HG2 | 1:24:A:ALA:HB3 | 4 | 0.66 | 0.24 | 0.55 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:18:A:ILE:HB | 4 | 0.66 | 0.24 | 0.55 |
| (1,3319) | 1:61:A:VAL:HG22 | 1:65:A:ASN:HB2 | 4 | 0.54 | 0.09 | 0.56 |
| (1,3319) | 1:61:A:VAL:HG22 | 1:65:A:ASN:HB3 | 4 | 0.54 | 0.09 | 0.56 |
| (1,3319) | 1:61:A:VAL:HG11 | 1:65:A:ASN:HB2 | 4 | 0.54 | 0.09 | 0.56 |
| (1,3319) | 1:61:A:VAL:HG11 | 1:65:A:ASN:HB3 | 4 | 0.54 | 0.09 | 0.56 |
| (1,3319) | 1:61:A:VAL:HG23 | 1:65:A:ASN:HB2 | 4 | 0.54 | 0.09 | 0.56 |
| (1,3319) | 1:61:A:VAL:HG23 | 1:65:A:ASN:HB3 | 4 | 0.54 | 0.09 | 0.56 |
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE21 | 4 | 0.5 | 0.2 | 0.5 |
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE22 | 4 | 0.5 | 0.2 | 0.5 |
| (1,1078) | 1:56:A:ALA:H | 1:50:A:ARG:HE | 4 | 0.5 | 0.2 | 0.5 |
| (1,3561) | 1:111:A:ARG:HD3 | 1:111:A:ARG:HA | 4 | 0.43 | 0.07 | 0.4 |
| (1,3561) | 1:50:A:ARG:HD2 | 1:50:A:ARG:HA | 4 | 0.43 | 0.07 | 0.4 |
| (1,3561) | 1:50:A:ARG:HD3 | 1:50:A:ARG:HA | 4 | 0.43 | 0.07 | 0.4 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD2 | 4 | 0.42 | 0.28 | 0.38 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD3 | 4 | 0.42 | 0.28 | 0.38 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD11 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD12 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD13 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD21 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD22 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD23 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD11 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD12 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD13 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD21 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD22 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD23 | 4 | 0.36 | 0.07 | 0.34 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG21 | 4 | 0.35 | 0.18 | 0.28 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG22 | 4 | 0.35 | 0.18 | 0.28 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG23 | 4 | 0.35 | 0.18 | 0.28 |
| (1,3707) | 1:86:A:TYR:HB2 | 1:43:A:ILE:HG21 | 4 | 0.35 | 0.18 | 0.28 |
| (1,3707) | 1:86:A:TYR:HB2 | 1:43:A:ILE:HG22 | 4 | 0.35 | 0.18 | 0.28 |
| (1,3707) | 1:86:A:TYR:HB2 | 1:43:A:ILE:HG23 | 4 | 0.35 | 0.18 | 0.28 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 4 | 0.35 | 0.18 | 0.28 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 4 | 0.35 | 0.18 | 0.28 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB2 | 4 | 0.35 | 0.16 | 0.38 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB3 | 4 | 0.35 | 0.16 | 0.38 |
| (1,1113) | 1:65:A:ASN:HD21 | 1:47:A:VAL:HB | 4 | 0.32 | 0.12 | 0.32 |
| (1,3583) | 1:74:A:VAL:HG23 | 1:44:A:ALA:HA | 4 | 0.32 | 0.1 | 0.32 |
| (1,3583) | 1:74:A:VAL:HG22 | 1:44:A:ALA:HA | 4 | 0.32 | 0.1 | 0.32 |
| (1,3583) | 1:74:A:VAL:HG21 | 1:44:A:ALA:HA | 4 | 0.32 | 0.1 | 0.32 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3645) | 1:25:A:LEU:HD11 | 1:180:A:SER:H | 4 | 0.3 | 0.1 | 0.28 |
| (1,3645) | 1:94:A:LEU:HD11 | 1:40:A:SER:H | 4 | 0.3 | 0.1 | 0.28 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD2 | 4 | 0.29 | 0.17 | 0.21 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD3 | 4 | 0.29 | 0.17 | 0.21 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD2 | 4 | 0.29 | 0.17 | 0.21 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD3 | 4 | 0.29 | 0.17 | 0.21 |
| (1,3421) | 1:22:A:ALA:HA | 1:191:A:PRO:HD2 | 4 | 0.29 | 0.17 | 0.21 |
| (1,3421) | 1:22:A:ALA:HA | 1:191:A:PRO:HD3 | 4 | 0.29 | 0.17 | 0.21 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG11 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG12 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG13 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG21 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG22 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG23 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD11 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD12 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD13 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD21 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD22 | 4 | 0.28 | 0.04 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD23 | 4 | 0.28 | 0.04 | 0.28 |
| (1,1039) | 1:90:A:PHE:H | 1:18:A:ILE:HB | 4 | 0.27 | 0.09 | 0.24 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG11 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG12 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG13 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG21 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG22 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG23 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG11 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG12 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG13 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG21 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG22 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG23 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG11 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG12 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG13 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG21 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG22 | 4 | 0.27 | 0.14 | 0.23 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG23 | 4 | 0.27 | 0.14 | 0.23 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB2 | 4 | 0.26 | 0.13 | 0.24 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB3 | 4 | 0.26 | 0.13 | 0.24 |
| (1,999) | 1:134:A:GLY:HA2 | 1:132:A:ASP:H | 4 | 0.26 | 0.07 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,999) | 1:134:A:GLY:HA3 | 1:132:A:ASP:H | 4 | 0.26 | 0.07 | 0.25 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB1 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB2 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB3 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:96:A:ASN:HB3 | 1:124:A:ALA:HB1 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:96:A:ASN:HB3 | 1:124:A:ALA:HB2 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:96:A:ASN:HB3 | 1:124:A:ALA:HB3 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:131:A:VAL:HB | 1:51:A:ALA:HB1 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:131:A:VAL:HB | 1:51:A:ALA:HB2 | 4 | 0.25 | 0.04 | 0.26 |
| (1,3587) | 1:131:A:VAL:HB | 1:51:A:ALA:HB3 | 4 | 0.25 | 0.04 | 0.26 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD11 | 4 | 0.23 | 0.04 | 0.24 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD12 | 4 | 0.23 | 0.04 | 0.24 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD13 | 4 | 0.23 | 0.04 | 0.24 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD21 | 4 | 0.23 | 0.04 | 0.24 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD22 | 4 | 0.23 | 0.04 | 0.24 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD23 | 4 | 0.23 | 0.04 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD2 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD3 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD2 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD3 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD2 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD3 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD2 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD3 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD2 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD3 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD2 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD3 | 4 | 0.21 | 0.02 | 0.21 |
| (1,3095) | 1:146:A:PHE:HB2 | 1:150:A:SER:HA | 4 | 0.21 | 0.09 | 0.18 |
| (1,3095) | 1:146:A:PHE:HB3 | 1:150:A:SER:HA | 4 | 0.21 | 0.09 | 0.18 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG2 | 4 | 0.2 | 0.09 | 0.16 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG3 | 4 | 0.2 | 0.09 | 0.16 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG2 | 4 | 0.2 | 0.09 | 0.16 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG3 | 4 | 0.2 | 0.09 | 0.16 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD11 | 4 | 0.19 | 0.05 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD12 | 4 | 0.19 | 0.05 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD13 | 4 | 0.19 | 0.05 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD21 | 4 | 0.19 | 0.05 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD22 | 4 | 0.19 | 0.05 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD23 | 4 | 0.19 | 0.05 | 0.18 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB2 | 4 | 0.19 | 0.05 | 0.19 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB3 | 4 | 0.19 | 0.05 | 0.19 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1028) | 1:71:A:VAL:H | 1:66:A:LEU:HA | 4 | 0.19 | 0.06 | 0.19 |
| (1,1028) | 1:71:A:VAL:H | 1:72:A:GLN:HA | 4 | 0.19 | 0.06 | 0.19 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB2 | 4 | 0.18 | 0.11 | 0.12 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB3 | 4 | 0.18 | 0.11 | 0.12 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG11 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG12 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG13 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG21 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG22 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG23 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG11 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG12 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG13 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG21 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG22 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG23 | 4 | 0.18 | 0.04 | 0.2 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD2 | 4 | 0.17 | 0.03 | 0.17 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD3 | 4 | 0.17 | 0.03 | 0.17 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA2 | 4 | 0.16 | 0.02 | 0.17 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA3 | 4 | 0.16 | 0.02 | 0.17 |
| (1,897) | 1:156:A:TYR:HA | 1:160:A:SER:H | 4 | 0.16 | 0.09 | 0.12 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG21 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG22 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG23 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG21 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG22 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG23 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG21 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG22 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG23 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG21 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG22 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG23 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG21 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG22 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG23 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG21 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG22 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG23 | 4 | 0.15 | 0.05 | 0.14 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG11 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG12 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG13 | 4 | 0.15 | 0.03 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG21 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG22 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG23 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG11 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG12 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG13 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG21 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG22 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG23 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE21 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE22 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE21 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE22 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE21 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE22 | 4 | 0.15 | 0.03 | 0.15 |
| (1,221) | 1:2:A:GLY:H | 1:45:A:SER:HA | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD11 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD12 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD13 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD21 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD22 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD23 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD11 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD12 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD13 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD21 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD23 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD11 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD12 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD13 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD21 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD22 | 4 | 0.15 | 0.01 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD23 | 4 | 0.15 | 0.01 | 0.15 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG2 | 4 | 0.15 | 0.03 | 0.15 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG3 | 4 | 0.15 | 0.03 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG21 | 4 | 0.15 | 0.03 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG22 | 4 | 0.15 | 0.03 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG23 | 4 | 0.15 | 0.03 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG21 | 4 | 0.15 | 0.03 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG22 | 4 | 0.15 | 0.03 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG23 | 4 | 0.15 | 0.03 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG21 | 4 | 0.15 | 0.03 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG22 | 4 | 0.15 | 0.03 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG23 | 4 | 0.15 | 0.03 | 0.16 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD11 | 4 | 0.14 | 0.03 | 0.14 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD12 | 4 | 0.14 | 0.03 | 0.14 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD13 | 4 | 0.14 | 0.03 | 0.14 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD21 | 4 | 0.14 | 0.03 | 0.14 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD22 | 4 | 0.14 | 0.03 | 0.14 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD23 | 4 | 0.14 | 0.03 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB2 | 4 | 0.14 | 0.0 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB3 | 4 | 0.14 | 0.0 | 0.14 |
| (1,2241) | 1:58:A:THR:HG21 | 1:61:A:VAL:HB | 4 | 0.14 | 0.03 | 0.14 |
| (1,2241) | 1:58:A:THR:HG22 | 1:61:A:VAL:HB | 4 | 0.14 | 0.03 | 0.14 |
| (1,2241) | 1:58:A:THR:HG23 | 1:61:A:VAL:HB | 4 | 0.14 | 0.03 | 0.14 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD21 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD22 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD21 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD22 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD21 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD22 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD21 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD22 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD21 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD22 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD21 | 4 | 0.14 | 0.02 | 0.14 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD22 | 4 | 0.14 | 0.02 | 0.14 |
| (1,801) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 4 | 0.13 | 0.01 | 0.14 |
| (1,1660) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 4 | 0.13 | 0.01 | 0.14 |
| (1,268) | 1:50:A:ARG:HG2 | 1:53:A:GLN:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,268) | 1:50:A:ARG:HG3 | 1:53:A:GLN:H | 4 | 0.13 | 0.02 | 0.12 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD2 | 4 | 0.13 | 0.01 | 0.13 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 4 | 0.13 | 0.01 | 0.13 |
| (1,276) | 1:50:A:ARG:HB2 | 1:54:A:SER:H | 4 | 0.12 | 0.04 | 0.11 |
| (1,276) | 1:50:A:ARG:HB3 | 1:54:A:SER:H | 4 | 0.12 | 0.04 | 0.11 |
| (1,2492) | 1:77:A:LEU:HD11 | 1:86:A:TYR:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD12 | 1:86:A:TYR:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD13 | 1:86:A:TYR:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD21 | 1:86:A:TYR:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD22 | 1:86:A:TYR:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD23 | 1:86:A:TYR:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB1 | 4 | 0.12 | 0.02 | 0.12 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB2 | 4 | 0.12 | 0.02 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB3 | 4 | 0.12 | 0.02 | 0.12 |
| (1,1281) | 1:33:A:THR:HB | 1:34:A:VAL:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,1989) | 1:33:A:THR:HB | 1:34:A:VAL:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB2 | 4 | 0.12 | 0.01 | 0.12 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB3 | 4 | 0.12 | 0.01 | 0.12 |
| (1,1777) | 1:165:A:SER:H | 1:165:A:SER:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,1777) | 1:153:A:SER:H | 1:153:A:SER:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,2835) | 1:110:A:SER:HA | 1:117:A:LEU:HA | 4 | 0.12 | 0.02 | 0.11 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD11 | 4 | 0.12 | 0.0 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD12 | 4 | 0.12 | 0.0 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD13 | 4 | 0.12 | 0.0 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD21 | 4 | 0.12 | 0.0 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD22 | 4 | 0.12 | 0.0 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD23 | 4 | 0.12 | 0.0 | 0.12 |
| (1,1957) | 1:30:A:THR:HG21 | 1:31:A:LEU:H | 4 | 0.11 | 0.0 | 0.11 |
| (1,1957) | 1:30:A:THR:HG22 | 1:31:A:LEU:H | 4 | 0.11 | 0.0 | 0.11 |
| (1,1957) | 1:30:A:THR:HG23 | 1:31:A:LEU:H | 4 | 0.11 | 0.0 | 0.11 |
| (1,3214) | 1:14:A:SER:HB2 | 1:18:A:ILE:HD11 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB2 | 1:18:A:ILE:HD12 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB2 | 1:18:A:ILE:HD13 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD11 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD12 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD13 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD21 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD22 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD23 | 3 | 0.32 | 0.17 | 0.25 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB2 | 3 | 0.27 | 0.03 | 0.27 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB3 | 3 | 0.27 | 0.03 | 0.27 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB2 | 3 | 0.27 | 0.03 | 0.27 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB3 | 3 | 0.27 | 0.03 | 0.27 |
| (1,3374) | 1:93:A:ALA:HB3 | 1:90:A:PHE:HA | 3 | 0.26 | 0.07 | 0.27 |
| (1,3374) | 1:93:A:ALA:HB2 | 1:90:A:PHE:HA | 3 | 0.26 | 0.07 | 0.27 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG21 | 3 | 0.26 | 0.09 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG22 | 3 | 0.26 | 0.09 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG23 | 3 | 0.26 | 0.09 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG21 | 3 | 0.26 | 0.09 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG22 | 3 | 0.26 | 0.09 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG23 | 3 | 0.26 | 0.09 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD11 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD12 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD13 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD21 | 3 | 0.25 | 0.13 | 0.23 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD22 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD23 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD11 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD12 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD13 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD21 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD22 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD23 | 3 | 0.25 | 0.13 | 0.23 |
| (1,3509) | 1:170:A:THR:HA | 1:170:A:THR:HB | 3 | 0.23 | 0.0 | 0.23 |
| (1,3509) | 1:10:A:THR:HA | 1:10:A:THR:HB | 3 | 0.23 | 0.0 | 0.23 |
| (1,3322) | 1:108:A:LEU:HD22 | 1:107:A:THR:HB | 3 | 0.22 | 0.04 | 0.22 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB2 | 3 | 0.22 | 0.01 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB3 | 3 | 0.22 | 0.01 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB2 | 3 | 0.22 | 0.01 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB3 | 3 | 0.22 | 0.01 | 0.21 |
| (1,3543) | 1:17:A:LEU:HD13 | 1:93:A:ALA:HA | 3 | 0.21 | 0.13 | 0.14 |
| (1,3543) | 1:17:A:LEU:HD11 | 1:93:A:ALA:HA | 3 | 0.21 | 0.13 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB1 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB2 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB3 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB1 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB2 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB3 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB1 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB2 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB3 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB1 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB2 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB3 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB1 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB2 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB3 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB1 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB2 | 3 | 0.21 | 0.09 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB3 | 3 | 0.21 | 0.09 | 0.16 |
| (1,2869) | 1:55:A:LEU:HB2 | 1:120:A:VAL:HA | 3 | 0.2 | 0.05 | 0.17 |
| (1,2869) | 1:55:A:LEU:HB3 | 1:120:A:VAL:HA | 3 | 0.2 | 0.05 | 0.17 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD2 | 3 | 0.19 | 0.05 | 0.2 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD3 | 3 | 0.19 | 0.05 | 0.2 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 3 | 0.19 | 0.04 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 3 | 0.19 | 0.04 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 3 | 0.19 | 0.04 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 3 | 0.19 | 0.04 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB2 | 3 | 0.19 | 0.04 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB3 | 3 | 0.19 | 0.04 | 0.17 |
| (1,3617) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HB2 | 3 | 0.19 | 0.05 | 0.21 |
| (1,3617) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HB3 | 3 | 0.19 | 0.05 | 0.21 |
| (1,3617) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HB2 | 3 | 0.19 | 0.05 | 0.21 |
| (1,3617) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HB3 | 3 | 0.19 | 0.05 | 0.21 |
| (1,927) | 1:179:A:PRO:HD2 | 1:187:A:GLY:H | 3 | 0.19 | 0.05 | 0.17 |
| (1,927) | 1:179:A:PRO:HD3 | 1:187:A:GLY:H | 3 | 0.19 | 0.05 | 0.17 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB2 | 3 | 0.18 | 0.05 | 0.15 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB3 | 3 | 0.18 | 0.05 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HA | 3 | 0.18 | 0.06 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 3 | 0.18 | 0.06 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 3 | 0.18 | 0.06 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HA | 3 | 0.18 | 0.06 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HA | 3 | 0.18 | 0.06 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HA | 3 | 0.18 | 0.06 | 0.15 |
| (1,11) | 1:4:A:GLN:H | 1:8:A:GLY:H | 3 | 0.18 | 0.03 | 0.2 |
| (1,917) | 1:161:A:ALA:H | 1:177:A:THR:HB | 3 | 0.18 | 0.06 | 0.18 |
| (1,893) | 1:153:A:SER:HB2 | 1:158:A:GLN:H | 3 | 0.18 | 0.04 | 0.2 |
| (1,893) | 1:153:A:SER:HB3 | 1:158:A:GLN:H | 3 | 0.18 | 0.04 | 0.2 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD1 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD2 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD1 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD2 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD1 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD2 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD1 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD2 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD1 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD2 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD1 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD2 | 3 | 0.18 | 0.04 | 0.16 |
| (1,2970) | 1:37:A:THR:HA | 1:131:A:VAL:HB | 3 | 0.18 | 0.05 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB2 | 3 | 0.17 | 0.04 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB3 | 3 | 0.17 | 0.04 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB2 | 3 | 0.17 | 0.04 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB3 | 3 | 0.17 | 0.04 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB2 | 3 | 0.17 | 0.04 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB3 | 3 | 0.17 | 0.04 | 0.18 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA2 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA3 | 3 | 0.17 | 0.06 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA2 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA3 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA2 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA3 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA2 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA3 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA2 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA3 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA2 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA3 | 3 | 0.17 | 0.06 | 0.14 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD11 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD12 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD13 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD21 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD22 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD23 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD11 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD12 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD13 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD21 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD22 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD23 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD11 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD12 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD13 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD21 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD22 | 3 | 0.17 | 0.08 | 0.13 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD23 | 3 | 0.17 | 0.08 | 0.13 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB2 | 3 | 0.17 | 0.04 | 0.19 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB3 | 3 | 0.17 | 0.04 | 0.19 |
| (1,885) | 1:154:A:ALA:HA | 1:156:A:TYR:H | 3 | 0.16 | 0.04 | 0.18 |
| (1,352) | 1:66:A:LEU:HG | 1:67:A:ALA:H | 3 | 0.16 | 0.04 | 0.18 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB1 | 3 | 0.16 | 0.02 | 0.15 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB2 | 3 | 0.16 | 0.02 | 0.15 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB3 | 3 | 0.16 | 0.02 | 0.15 |
| (1,3368) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 3 | 0.16 | 0.02 | 0.15 |
| (1,3368) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 3 | 0.16 | 0.02 | 0.15 |
| (1,3368) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 3 | 0.16 | 0.02 | 0.15 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 3 | 0.16 | 0.04 | 0.15 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 3 | 0.16 | 0.04 | 0.15 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB2 | 3 | 0.16 | 0.05 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB3 | 3 | 0.16 | 0.05 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB2 | 3 | 0.16 | 0.05 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB3 | 3 | 0.16 | 0.05 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG11 | 1:93:A:ALA:HA | 3 | 0.16 | 0.06 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG12 | 1:93:A:ALA:HA | 3 | 0.16 | 0.06 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG13 | 1:93:A:ALA:HA | 3 | 0.16 | 0.06 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG21 | 1:93:A:ALA:HA | 3 | 0.16 | 0.06 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG22 | 1:93:A:ALA:HA | 3 | 0.16 | 0.06 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG23 | 1:93:A:ALA:HA | 3 | 0.16 | 0.06 | 0.12 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 3 | 0.16 | 0.06 | 0.12 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 3 | 0.16 | 0.06 | 0.12 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 3 | 0.16 | 0.06 | 0.12 |
| (1,1023) | 1:164:A:THR:HA | 1:166:A:GLY:H | 3 | 0.15 | 0.03 | 0.15 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD21 | 3 | 0.15 | 0.02 | 0.15 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD22 | 3 | 0.15 | 0.02 | 0.15 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD21 | 3 | 0.15 | 0.02 | 0.15 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD22 | 3 | 0.15 | 0.02 | 0.15 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG2 | 3 | 0.15 | 0.05 | 0.13 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG3 | 3 | 0.15 | 0.05 | 0.13 |
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG2 | 3 | 0.15 | 0.05 | 0.13 |
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG3 | 3 | 0.15 | 0.05 | 0.13 |
| (1,3003) | 1:131:A:VAL:HG11 | 1:136:A:VAL:HB | 3 | 0.15 | 0.04 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG12 | 1:136:A:VAL:HB | 3 | 0.15 | 0.04 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG13 | 1:136:A:VAL:HB | 3 | 0.15 | 0.04 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG21 | 1:136:A:VAL:HB | 3 | 0.15 | 0.04 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG22 | 1:136:A:VAL:HB | 3 | 0.15 | 0.04 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG23 | 1:136:A:VAL:HB | 3 | 0.15 | 0.04 | 0.15 |
| (1,609) | 1:101:A:ASN:H | 1:105:A:ILE:H | 3 | 0.14 | 0.03 | 0.15 |
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 3 | 0.14 | 0.02 | 0.13 |
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 3 | 0.14 | 0.02 | 0.13 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 3 | 0.14 | 0.02 | 0.13 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 3 | 0.14 | 0.02 | 0.13 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB1 | 3 | 0.14 | 0.03 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB2 | 3 | 0.14 | 0.03 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB3 | 3 | 0.14 | 0.03 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:123:A:ALA:HB1 | 3 | 0.14 | 0.03 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:123:A:ALA:HB2 | 3 | 0.14 | 0.03 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:123:A:ALA:HB3 | 3 | 0.14 | 0.03 | 0.12 |
| (1,315) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 3 | 0.13 | 0.02 | 0.14 |
| (1,315) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 3 | 0.13 | 0.02 | 0.14 |
| (1,1127) | 1:163:A:SER:H | 1:162:A:SER:HA | 3 | 0.13 | 0.01 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG11 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG12 | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG13 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG21 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG22 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG23 | 3 | 0.13 | 0.01 | 0.13 |
| (1,1403) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 3 | 0.13 | 0.02 | 0.14 |
| (1,1403) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 3 | 0.13 | 0.02 | 0.14 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG21 | 3 | 0.13 | 0.02 | 0.13 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG22 | 3 | 0.13 | 0.02 | 0.13 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG23 | 3 | 0.13 | 0.02 | 0.13 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG21 | 3 | 0.13 | 0.02 | 0.13 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG22 | 3 | 0.13 | 0.02 | 0.13 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG23 | 3 | 0.13 | 0.02 | 0.13 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD2 | 3 | 0.13 | 0.02 | 0.12 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD3 | 3 | 0.13 | 0.02 | 0.12 |
| (1,946) | 1:196:A:GLY:H | 1:197:A:PHE:HA | 3 | 0.13 | 0.02 | 0.12 |
| (1,2961) | 1:38:A:GLY:HA2 | 1:130:A:ASN:HA | 3 | 0.13 | 0.03 | 0.11 |
| (1,2961) | 1:38:A:GLY:HA3 | 1:130:A:ASN:HA | 3 | 0.13 | 0.03 | 0.11 |
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD2 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD3 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD2 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD3 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD2 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD3 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD2 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD3 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD2 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD3 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD2 | 3 | 0.13 | 0.02 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD3 | 3 | 0.13 | 0.02 | 0.14 |
| (1,258) | 1:49:A:GLN:HB2 | 1:51:A:ALA:H | 3 | 0.13 | 0.02 | 0.12 |
| (1,258) | 1:49:A:GLN:HB3 | 1:51:A:ALA:H | 3 | 0.13 | 0.02 | 0.12 |
| (1,332) | 1:61:A:VAL:HA | 1:64:A:ASN:H | 3 | 0.13 | 0.02 | 0.12 |
| (1,876) | 1:148:A:SER:H | 1:149:A:THR:H | 3 | 0.13 | 0.01 | 0.12 |
| (1,824) | 1:37:A:THR:HG21 | 1:136:A:VAL:H | 3 | 0.12 | 0.01 | 0.11 |
| (1,824) | 1:37:A:THR:HG22 | 1:136:A:VAL:H | 3 | 0.12 | 0.01 | 0.11 |
| (1,824) | 1:37:A:THR:HG23 | 1:136:A:VAL:H | 3 | 0.12 | 0.01 | 0.11 |
| (1,648) | 1:108:A:LEU:HD11 | 1:110:A:SER:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,648) | 1:108:A:LEU:HD12 | 1:110:A:SER:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,648) | 1:108:A:LEU:HD13 | 1:110:A:SER:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,648) | 1:108:A:LEU:HD21 | 1:110:A:SER:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,648) | 1:108:A:LEU:HD22 | 1:110:A:SER:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,648) | 1:108:A:LEU:HD23 | 1:110:A:SER:H | 3 | 0.11 | 0.0 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,256) | 1:50:A:ARG:H | 1:51:A:ALA:H | 3 | 0.11 | 0.01 | 0.1 |
| (1,257) | 1:50:A:ARG:H | 1:51:A:ALA:H | 3 | 0.11 | 0.01 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB1 | 3 | 0.11 | 0.01 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB2 | 3 | 0.11 | 0.01 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB3 | 3 | 0.11 | 0.01 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB1 | 3 | 0.11 | 0.01 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB2 | 3 | 0.11 | 0.01 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB3 | 3 | 0.11 | 0.01 | 0.1 |
| (1,6) | 1:6:A:GLY:HA2 | 1:7:A:PHE:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,6) | 1:6:A:GLY:HA3 | 1:7:A:PHE:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,2670) | 1:103:A:SER:H | 1:104:A:ASN:HA | 3 | 0.11 | 0.0 | 0.11 |
| (1,3213) | 1:129:A:ILE:HD13 | 1:50:A:ARG:HG2 | 2 | 0.7 | 0.07 | 0.7 |
| (1,3213) | 1:129:A:ILE:HD13 | 1:50:A:ARG:HG3 | 2 | 0.7 | 0.07 | 0.7 |
| (1,3213) | 1:129:A:ILE:HD12 | 1:50:A:ARG:HG2 | 2 | 0.7 | 0.07 | 0.7 |
| (1,3213) | 1:129:A:ILE:HD12 | 1:50:A:ARG:HG3 | 2 | 0.7 | 0.07 | 0.7 |
| (1,3355) | 1:28:A:THR:HG22 | 1:34:A:VAL:HB | 2 | 0.62 | 0.46 | 0.62 |
| (1,3355) | 1:28:A:THR:HG23 | 1:34:A:VAL:HB | 2 | 0.62 | 0.46 | 0.62 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD11 | 2 | 0.52 | 0.02 | 0.52 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD12 | 2 | 0.52 | 0.02 | 0.52 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD13 | 2 | 0.52 | 0.02 | 0.52 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD21 | 2 | 0.52 | 0.02 | 0.52 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD22 | 2 | 0.52 | 0.02 | 0.52 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD23 | 2 | 0.52 | 0.02 | 0.52 |
| (1,3513) | 1:85:A:ALA:HB2 | 1:81:A:SER:HB2 | 2 | 0.52 | 0.03 | 0.52 |
| (1,3513) | 1:85:A:ALA:HB2 | 1:81:A:SER:HB3 | 2 | 0.52 | 0.03 | 0.52 |
| (1,3513) | 1:85:A:ALA:HB1 | 1:81:A:SER:HB2 | 2 | 0.52 | 0.03 | 0.52 |
| (1,3513) | 1:85:A:ALA:HB1 | 1:81:A:SER:HB3 | 2 | 0.52 | 0.03 | 0.52 |
| (1,3748) | 1:50:A:ARG:HD2 | 1:55:A:LEU:HA | 2 | 0.44 | 0.08 | 0.44 |
| (1,3748) | 1:36:A:ARG:HD2 | 1:91:A:SER:HB2 | 2 | 0.44 | 0.08 | 0.44 |
| (1,3748) | 1:36:A:ARG:HD2 | 1:91:A:SER:HB3 | 2 | 0.44 | 0.08 | 0.44 |
| (1,3820) | 1:101:A:ASN:HB2 | 1:104:A:ASN:HB2 | 2 | 0.42 | 0.06 | 0.42 |
| (1,3820) | 1:101:A:ASN:HB2 | 1:104:A:ASN:HB3 | 2 | 0.42 | 0.06 | 0.42 |
| (1,1143) | 1:127:A:LEU:H | 1:124:A:ALA:HB1 | 2 | 0.42 | 0.27 | 0.42 |
| (1,1143) | 1:127:A:LEU:H | 1:124:A:ALA:HB2 | 2 | 0.42 | 0.27 | 0.42 |
| (1,1143) | 1:127:A:LEU:H | 1:124:A:ALA:HB3 | 2 | 0.42 | 0.27 | 0.42 |
| (1,1143) | 1:127:A:LEU:H | 1:123:A:ALA:HB1 | 2 | 0.42 | 0.27 | 0.42 |
| (1,1143) | 1:127:A:LEU:H | 1:123:A:ALA:HB2 | 2 | 0.42 | 0.27 | 0.42 |
| (1,1143) | 1:127:A:LEU:H | 1:123:A:ALA:HB3 | 2 | 0.42 | 0.27 | 0.42 |
| (1,1976) | 1:32:A:ARG:HG2 | 1:33:A:THR:HA | 2 | 0.42 | 0.31 | 0.42 |
| (1,1976) | 1:32:A:ARG:HG3 | 1:33:A:THR:HA | 2 | 0.42 | 0.31 | 0.42 |
| (1,3106) | 1:154:A:ALA:HB1 | 1:158:A:GLN:HB2 | 2 | 0.4 | 0.05 | 0.4 |
| (1,3106) | 1:154:A:ALA:HB1 | 1:158:A:GLN:HB3 | 2 | 0.4 | 0.05 | 0.4 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,3106) | 1:154:A:ALA:HB2 | 1:158:A:GLN:HB2 | 2 | 0.4 | 0.05 | 0.4 |
| (1,3106) | 1:154:A:ALA:HB2 | 1:158:A:GLN:HB3 | 2 | 0.4 | 0.05 | 0.4 |
| (1,3106) | 1:154:A:ALA:HB3 | 1:158:A:GLN:HB2 | 2 | 0.4 | 0.05 | 0.4 |
| (1,3106) | 1:154:A:ALA:HB3 | 1:158:A:GLN:HB3 | 2 | 0.4 | 0.05 | 0.4 |
| (1,3756) | 1:156:A:TYR:HB2 | 1:157:A:SER:HA | 2 | 0.37 | 0.16 | 0.37 |
| (1,3173) | 1:177:A:THR:HG21 | 1:190:A:ALA:HA | 2 | 0.36 | 0.2 | 0.36 |
| (1,3173) | 1:177:A:THR:HG22 | 1:190:A:ALA:HA | 2 | 0.36 | 0.2 | 0.36 |
| (1,3173) | 1:177:A:THR:HG23 | 1:190:A:ALA:HA | 2 | 0.36 | 0.2 | 0.36 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB1 | 2 | 0.35 | 0.11 | 0.35 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB2 | 2 | 0.35 | 0.11 | 0.35 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB3 | 2 | 0.35 | 0.11 | 0.35 |
| (1,1075) | 1:48:A:VAL:H | 1:73:A:ALA:HB1 | 2 | 0.32 | 0.2 | 0.32 |
| (1,1075) | 1:48:A:VAL:H | 1:73:A:ALA:HB2 | 2 | 0.32 | 0.2 | 0.32 |
| (1,1075) | 1:48:A:VAL:H | 1:73:A:ALA:HB3 | 2 | 0.32 | 0.2 | 0.32 |
| (1,1075) | 1:48:A:VAL:H | 1:56:A:ALA:HB1 | 2 | 0.32 | 0.2 | 0.32 |
| (1,1075) | 1:48:A:VAL:H | 1:56:A:ALA:HB2 | 2 | 0.32 | 0.2 | 0.32 |
| (1,1075) | 1:48:A:VAL:H | 1:56:A:ALA:HB3 | 2 | 0.32 | 0.2 | 0.32 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD11 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD12 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD13 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD21 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD22 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD23 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD11 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD12 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD13 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD21 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD22 | 2 | 0.3 | 0.12 | 0.3 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD23 | 2 | 0.3 | 0.12 | 0.3 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG11 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG12 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG13 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG21 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG22 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG23 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG11 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG12 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG13 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG21 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG22 | 2 | 0.29 | 0.16 | 0.29 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG23 | 2 | 0.29 | 0.16 | 0.29 |
| (1,919) | 1:180:A:SER:H | 1:180:A:SER:HB2 | 2 | 0.28 | 0.1 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,919) | 1:180:A:SER:H | 1:180:A:SER:HB3 | 2 | 0.28 | 0.1 | 0.28 |
| (1,961) | 1:10:A:THR:H | 1:117:A:LEU:H | 2 | 0.28 | 0.06 | 0.28 |
| (1,961) | 1:10:A:THR:H | 1:113:A:LEU:H | 2 | 0.28 | 0.06 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG21 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG22 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG23 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG21 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG22 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG23 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG21 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG22 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG23 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG21 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG22 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG23 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG21 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG22 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG23 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG21 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG22 | 2 | 0.28 | 0.02 | 0.28 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG23 | 2 | 0.28 | 0.02 | 0.28 |
| (1,141) | 1:29:A:SER:H | 1:32:A:ARG:HD2 | 2 | 0.26 | 0.03 | 0.26 |
| (1,141) | 1:29:A:SER:H | 1:32:A:ARG:HD3 | 2 | 0.26 | 0.03 | 0.26 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB1 | 2 | 0.26 | 0.03 | 0.26 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB2 | 2 | 0.26 | 0.03 | 0.26 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB3 | 2 | 0.26 | 0.03 | 0.26 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB1 | 2 | 0.26 | 0.03 | 0.26 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB2 | 2 | 0.26 | 0.03 | 0.26 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB3 | 2 | 0.26 | 0.03 | 0.26 |
| (1,925) | 1:185:A:PRO:HG2 | 1:186:A:LEU:H | 2 | 0.26 | 0.02 | 0.26 |
| (1,925) | 1:185:A:PRO:HG3 | 1:186:A:LEU:H | 2 | 0.26 | 0.02 | 0.26 |
| (1,3404) | 1:31:A:LEU:HD11 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD11 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD12 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD12 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD13 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD13 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD21 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD21 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD22 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD22 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:31:A:LEU:HD23 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3404) | 1:31:A:LEU:HD23 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HG2 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3404) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HG3 | 2 | 0.25 | 0.05 | 0.25 |
| (1,3559) | 1:156:A:TYR:HA | 1:155:A:SER:HB2 | 2 | 0.24 | 0.12 | 0.24 |
| (1,3559) | 1:156:A:TYR:HA | 1:155:A:SER:HB3 | 2 | 0.24 | 0.12 | 0.24 |
| (1,3913) | 1:99:A:VAL:HG11 | 1:95:A:PHE:HD1 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG11 | 1:95:A:PHE:HD2 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG12 | 1:95:A:PHE:HD1 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG12 | 1:95:A:PHE:HD2 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG13 | 1:95:A:PHE:HD1 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG13 | 1:95:A:PHE:HD2 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG21 | 1:95:A:PHE:HD1 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG21 | 1:95:A:PHE:HD2 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG22 | 1:95:A:PHE:HD1 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG22 | 1:95:A:PHE:HD2 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG23 | 1:95:A:PHE:HD1 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3913) | 1:99:A:VAL:HG23 | 1:95:A:PHE:HD2 | 2 | 0.23 | 0.05 | 0.23 |
| (1,3400) | 1:140:A:ILE:HD11 | 1:141:A:SER:HB2 | 2 | 0.23 | 0.02 | 0.23 |
| (1,3400) | 1:140:A:ILE:HD11 | 1:141:A:SER:HB3 | 2 | 0.23 | 0.02 | 0.23 |
| (1,3400) | 1:140:A:ILE:HD13 | 1:37:A:THR:HB | 2 | 0.23 | 0.02 | 0.23 |
| (1,3497) | 1:90:A:PHE:HA | 1:92:A:SER:HB2 | 2 | 0.22 | 0.02 | 0.22 |
| (1,3497) | 1:90:A:PHE:HA | 1:92:A:SER:HB3 | 2 | 0.22 | 0.02 | 0.22 |
| (1,928) | 1:178:A:GLY:HA2 | 1:187:A:GLY:H | 2 | 0.22 | 0.08 | 0.22 |
| (1,928) | 1:178:A:GLY:HA3 | 1:187:A:GLY:H | 2 | 0.22 | 0.08 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG11 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG12 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG13 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG21 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG22 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG23 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG23 | 1:37:A:THR:HG21 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG23 | 1:37:A:THR:HG22 | 2 | 0.22 | 0.1 | 0.22 |
| (1,3599) | 1:129:A:ILE:HG23 | 1:37:A:THR:HG23 | 2 | 0.22 | 0.1 | 0.22 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD11 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD12 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD13 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD21 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD22 | 2 | 0.21 | 0.04 | 0.21 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD23 | 2 | 0.21 | 0.04 | 0.21 |
| (1,892) | 1:153:A:SER:H | 1:158:A:GLN:HB2 | 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) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,892) | 1:153:A:SER:H | 1:158:A:GLN:HB3 | 2 | 0.2 | 0.06 | 0.2 |
| (1,3136) | 1:163:A:SER:HB2 | 1:175:A:PRO:HD2 | 2 | 0.2 | 0.01 | 0.2 |
| (1,3136) | 1:163:A:SER:HB2 | 1:175:A:PRO:HD3 | 2 | 0.2 | 0.01 | 0.2 |
| (1,3136) | 1:163:A:SER:HB3 | 1:175:A:PRO:HD2 | 2 | 0.2 | 0.01 | 0.2 |
| (1,3136) | 1:163:A:SER:HB3 | 1:175:A:PRO:HD3 | 2 | 0.2 | 0.01 | 0.2 |
| (1,365) | 1:68:A:ARG:HG2 | 1:69:A:PHE:H | 2 | 0.2 | 0.01 | 0.2 |
| (1,365) | 1:68:A:ARG:HG3 | 1:69:A:PHE:H | 2 | 0.2 | 0.01 | 0.2 |
| (1,2980) | 1:131:A:VAL:HG11 | 1:134:A:GLY:HA2 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG11 | 1:134:A:GLY:HA3 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG12 | 1:134:A:GLY:HA2 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG12 | 1:134:A:GLY:HA3 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG13 | 1:134:A:GLY:HA2 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG13 | 1:134:A:GLY:HA3 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG21 | 1:134:A:GLY:HA2 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG21 | 1:134:A:GLY:HA3 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG22 | 1:134:A:GLY:HA2 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG22 | 1:134:A:GLY:HA3 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG23 | 1:134:A:GLY:HA2 | 2 | 0.18 | 0.01 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG23 | 1:134:A:GLY:HA3 | 2 | 0.18 | 0.01 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG21 | 1:41:A:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG21 | 1:41:A:GLN:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG23 | 1:41:A:GLN:HG2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,3394) | 1:48:A:VAL:HG23 | 1:41:A:GLN:HG3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,875) | 1:148:A:SER:HB2 | 1:149:A:THR:H | 2 | 0.18 | 0.04 | 0.18 |
| (1,875) | 1:148:A:SER:HB3 | 1:149:A:THR:H | 2 | 0.18 | 0.04 | 0.18 |
| (1,2447) | 1:77:A:LEU:HB2 | 1:78:A:PRO:HG2 | 2 | 0.17 | 0.0 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB2 | 1:78:A:PRO:HG3 | 2 | 0.17 | 0.0 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB3 | 1:78:A:PRO:HG2 | 2 | 0.17 | 0.0 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB3 | 1:78:A:PRO:HG3 | 2 | 0.17 | 0.0 | 0.17 |
| (1,123) | 1:31:A:LEU:H | 1:31:A:LEU:HG | 2 | 0.17 | 0.01 | 0.17 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG11 | 2 | 0.17 | 0.05 | 0.17 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG12 | 2 | 0.17 | 0.05 | 0.17 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG13 | 2 | 0.17 | 0.05 | 0.17 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG21 | 2 | 0.17 | 0.05 | 0.17 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG22 | 2 | 0.17 | 0.05 | 0.17 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG23 | 2 | 0.17 | 0.05 | 0.17 |
| (1,3087) | 1:148:A:SER:HB2 | 1:149:A:THR:HB | 2 | 0.17 | 0.07 | 0.17 |
| (1,3087) | 1:148:A:SER:HB3 | 1:149:A:THR:HB | 2 | 0.17 | 0.07 | 0.17 |
| (1,945) | 1:194:A:GLN:HG2 | 1:196:A:GLY:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,945) | 1:194:A:GLN:HG3 | 1:196:A:GLY:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,555) | 1:99:A:VAL:H | 1:100:A:LEU:HG | 2 | 0.16 | 0.04 | 0.16 |
| (1,3185) | 1:20:A:ARG:HD2 | 1:191:A:PRO:HA | 2 | 0.16 | 0.04 | 0.16 |
| (1,3185) | 1:20:A:ARG:HD3 | 1:191:A:PRO:HA | 2 | 0.16 | 0.04 | 0.16 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB3 | 2 | 0.16 | 0.02 | 0.16 |
| (1,1002) | 1:92:A:SER:H | 1:21:A:VAL:HB | 2 | 0.16 | 0.05 | 0.16 |
| (1,3169) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HA | 2 | 0.16 | 0.03 | 0.16 |
| (1,3169) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HA | 2 | 0.16 | 0.03 | 0.16 |
| (1,3171) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HA | 2 | 0.16 | 0.03 | 0.16 |
| (1,3171) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HA | 2 | 0.16 | 0.03 | 0.16 |
| (1,3516) | 1:58:A:THR:HA | 1:59:A:LEU:HG | 2 | 0.16 | 0.05 | 0.16 |
| (1,312) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,312) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,313) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,313) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,1401) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,1401) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB3 | 2 | 0.16 | 0.02 | 0.16 |
| (1,362) | 1:66:A:LEU:HG | 1:68:A:ARG:H | 2 | 0.16 | 0.02 | 0.16 |
| (1,2520) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 2 | 0.15 | 0.01 | 0.15 |
| (1,2520) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 2 | 0.15 | 0.01 | 0.15 |
| (1,708) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,708) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,711) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.0 | 0.15 |
| (1,711) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.0 | 0.15 |
| (1,783) | 1:50:A:ARG:HD2 | 1:129:A:ILE:H | 2 | 0.15 | 0.04 | 0.15 |
| (1,783) | 1:50:A:ARG:HD3 | 1:129:A:ILE:H | 2 | 0.15 | 0.04 | 0.15 |
| (1,2846) | 1:117:A:LEU:HG | 1:118:A:ASN:HD21 | 2 | 0.15 | 0.03 | 0.15 |
| (1,2846) | 1:117:A:LEU:HG | 1:118:A:ASN:HD22 | 2 | 0.15 | 0.03 | 0.15 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG21 | 2 | 0.15 | 0.03 | 0.15 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG22 | 2 | 0.15 | 0.03 | 0.15 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG23 | 2 | 0.15 | 0.03 | 0.15 |
| (1,594) | 1:100:A:LEU:HD11 | 1:104:A:ASN:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,594) | 1:100:A:LEU:HD12 | 1:104:A:ASN:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,594) | 1:100:A:LEU:HD13 | 1:104:A:ASN:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,594) | 1:100:A:LEU:HD21 | 1:104:A:ASN:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,594) | 1:100:A:LEU:HD22 | 1:104:A:ASN:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,594) | 1:100:A:LEU:HD23 | 1:104:A:ASN:H | 2 | 0.15 | 0.03 | 0.15 |
| (1,778) | 1:128:A:GLY:H | 1:129:A:ILE:HG12 | 2 | 0.15 | 0.0 | 0.15 |
| (1,778) | 1:128:A:GLY:H | 1:129:A:ILE:HG13 | 2 | 0.15 | 0.0 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG11 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG12 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG13 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG21 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG22 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG23 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG11 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG12 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG13 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG21 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG22 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG23 | 2 | 0.15 | 0.02 | 0.15 |
| (1,2600) | 1:93:A:ALA:HB1 | 1:96:A:ASN:HB2 | 2 | 0.15 | 0.04 | 0.15 |
| (1,2600) | 1:93:A:ALA:HB1 | 1:96:A:ASN:HB3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,2600) | 1:93:A:ALA:HB2 | 1:96:A:ASN:HB2 | 2 | 0.15 | 0.04 | 0.15 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,2600) | 1:93:A:ALA:HB2 | 1:96:A:ASN:HB3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,2600) | 1:93:A:ALA:HB3 | 1:96:A:ASN:HB2 | 2 | 0.15 | 0.04 | 0.15 |
| (1,2600) | 1:93:A:ALA:HB3 | 1:96:A:ASN:HB3 | 2 | 0.15 | 0.04 | 0.15 |
| (1,2731) | 1:108:A:LEU:HG | 1:109:A:GLY:HA2 | 2 | 0.15 | 0.03 | 0.15 |
| (1,2731) | 1:108:A:LEU:HG | 1:109:A:GLY:HA3 | 2 | 0.15 | 0.03 | 0.15 |
| (1,3285) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3285) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3285) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3285) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3285) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3285) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3876) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3876) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3876) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3876) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3876) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 2 | 0.15 | 0.02 | 0.15 |
| (1,3876) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 2 | 0.15 | 0.02 | 0.15 |
| (1,1736) | 1:176:A:SER:HA | 1:177:A:THR:H | 2 | 0.14 | 0.04 | 0.14 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2287) | 1:66:A:LEU:HD11 | 1:67:A:ALA:HA | 2 | 0.14 | 0.03 | 0.14 |
| (1,2287) | 1:66:A:LEU:HD12 | 1:67:A:ALA:HA | 2 | 0.14 | 0.03 | 0.14 |
| (1,2287) | 1:66:A:LEU:HD13 | 1:67:A:ALA:HA | 2 | 0.14 | 0.03 | 0.14 |
| (1,2287) | 1:66:A:LEU:HD21 | 1:67:A:ALA:HA | 2 | 0.14 | 0.03 | 0.14 |
| (1,2287) | 1:66:A:LEU:HD22 | 1:67:A:ALA:HA | 2 | 0.14 | 0.03 | 0.14 |
| (1,2287) | 1:66:A:LEU:HD23 | 1:67:A:ALA:HA | 2 | 0.14 | 0.03 | 0.14 |
| (1,3060) | 1:137:A:GLN:HG2 | 1:141:A:SER:HA | 2 | 0.14 | 0.01 | 0.14 |
| (1,3060) | 1:137:A:GLN:HG3 | 1:141:A:SER:HA | 2 | 0.14 | 0.01 | 0.14 |
| (1,106) | 1:27:A:ASN:H | 1:27:A:ASN:HD21 | 2 | 0.14 | 0.02 | 0.14 |
| (1,106) | 1:27:A:ASN:H | 1:27:A:ASN:HD22 | 2 | 0.14 | 0.02 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG11 | 2 | 0.14 | 0.01 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG12 | 2 | 0.14 | 0.01 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG13 | 2 | 0.14 | 0.01 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG21 | 2 | 0.14 | 0.01 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG22 | 2 | 0.14 | 0.01 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG23 | 2 | 0.14 | 0.01 | 0.14 |
| (1,561) | 1:22:A:ALA:H | 1:100:A:LEU:HA | 2 | 0.14 | 0.02 | 0.14 |
| (1,1868) | 1:18:A:ILE:HB | 1:19:A:SER:HB2 | 2 | 0.14 | 0.02 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1868) | 1:18:A:ILE:HB | 1:19:A:SER:HB3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB1 | 1:125:A:GLN:HG2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB1 | 1:125:A:GLN:HG3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HG2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HG3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HG2 | 2 | 0.14 | 0.01 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HG3 | 2 | 0.14 | 0.01 | 0.14 |
| (1,3122) | 1:20:A:ARG:HG2 | 1:171:A:GLY:HA2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,3122) | 1:20:A:ARG:HG2 | 1:171:A:GLY:HA3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,3122) | 1:20:A:ARG:HG3 | 1:171:A:GLY:HA2 | 2 | 0.14 | 0.02 | 0.14 |
| (1,3122) | 1:20:A:ARG:HG3 | 1:171:A:GLY:HA3 | 2 | 0.14 | 0.02 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3199) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG2 | 2 | 0.14 | 0.04 | 0.14 |
| (1,3200) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG3 | 2 | 0.14 | 0.04 | 0.14 |
| (1,524) | 1:37:A:THR:H | 1:95:A:PHE:HB2 | 2 | 0.13 | 0.02 | 0.13 |
| (1,524) | 1:37:A:THR:H | 1:95:A:PHE:HB3 | 2 | 0.13 | 0.02 | 0.13 |
| (1,598) | 1:96:A:ASN:HD21 | 1:104:A:ASN:HD21 | 2 | 0.13 | 0.02 | 0.13 |
| (1,598) | 1:96:A:ASN:HD21 | 1:104:A:ASN:HD22 | 2 | 0.13 | 0.02 | 0.13 |
| (1,598) | 1:96:A:ASN:HD22 | 1:104:A:ASN:HD21 | 2 | 0.13 | 0.02 | 0.13 |
| (1,598) | 1:96:A:ASN:HD22 | 1:104:A:ASN:HD22 | 2 | 0.13 | 0.02 | 0.13 |
| (1,940) | 1:191:A:PRO:HD2 | 1:193:A:GLY:H | 2 | 0.12 | 0.01 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,940) | 1:191:A:PRO:HD3 | 1:193:A:GLY:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,2720) | 1:107:A:THR:HG21 | 1:108:A:LEU:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,2720) | 1:107:A:THR:HG21 | 1:108:A:LEU:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,2720) | 1:107:A:THR:HG22 | 1:108:A:LEU:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,2720) | 1:107:A:THR:HG22 | 1:108:A:LEU:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,2720) | 1:107:A:THR:HG23 | 1:108:A:LEU:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,2720) | 1:107:A:THR:HG23 | 1:108:A:LEU:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,23) | 1:11:A:GLY:HA2 | 1:14:A:SER:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,23) | 1:11:A:GLY:HA3 | 1:14:A:SER:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,559) | 1:99:A:VAL:HB | 1:100:A:LEU:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,1551) | 1:99:A:VAL:HB | 1:100:A:LEU:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,2906) | 1:105:A:ILE:HG21 | 1:125:A:GLN:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2906) | 1:105:A:ILE:HG21 | 1:125:A:GLN:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2906) | 1:105:A:ILE:HG22 | 1:125:A:GLN:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2906) | 1:105:A:ILE:HG22 | 1:125:A:GLN:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2906) | 1:105:A:ILE:HG23 | 1:125:A:GLN:HG2 | 2 | 0.12 | 0.01 | 0.12 |
| (1,2906) | 1:105:A:ILE:HG23 | 1:125:A:GLN:HG3 | 2 | 0.12 | 0.01 | 0.12 |
| (1,3166) | 1:186:A:LEU:HD11 | 1:190:A:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,3166) | 1:186:A:LEU:HD12 | 1:190:A:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,3166) | 1:186:A:LEU:HD13 | 1:190:A:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,3166) | 1:186:A:LEU:HD21 | 1:190:A:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,3166) | 1:186:A:LEU:HD22 | 1:190:A:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,3166) | 1:186:A:LEU:HD23 | 1:190:A:ALA:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,101) | 1:27:A:ASN:H | 1:27:A:ASN:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,101) | 1:27:A:ASN:H | 1:27:A:ASN:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,633) | 1:14:A:SER:H | 1:108:A:LEU:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,633) | 1:14:A:SER:H | 1:108:A:LEU:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1257) | 1:27:A:ASN:H | 1:27:A:ASN:HB2 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1257) | 1:27:A:ASN:H | 1:27:A:ASN:HB3 | 2 | 0.12 | 0.02 | 0.12 |
| (1,1833) | 1:13:A:ALA:HA | 1:16:A:GLY:HA2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1833) | 1:13:A:ALA:HA | 1:16:A:GLY:HA3 | 2 | 0.12 | 0.0 | 0.12 |
| (1,69) | 1:21:A:VAL:HG11 | 1:22:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,69) | 1:21:A:VAL:HG12 | 1:22:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,69) | 1:21:A:VAL:HG13 | 1:22:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,69) | 1:21:A:VAL:HG21 | 1:22:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,69) | 1:21:A:VAL:HG22 | 1:22:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,69) | 1:21:A:VAL:HG23 | 1:22:A:ALA:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,913) | 1:169:A:TYR:H | 1:175:A:PRO:HD2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,913) | 1:169:A:TYR:H | 1:175:A:PRO:HD3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2484) | 1:83:A:THR:HG21 | 1:86:A:TYR:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,2484) | 1:83:A:THR:HG22 | 1:86:A:TYR:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,2484) | 1:83:A:THR:HG23 | 1:86:A:TYR:H | 2 | 0.11 | 0.0 | 0.11 |

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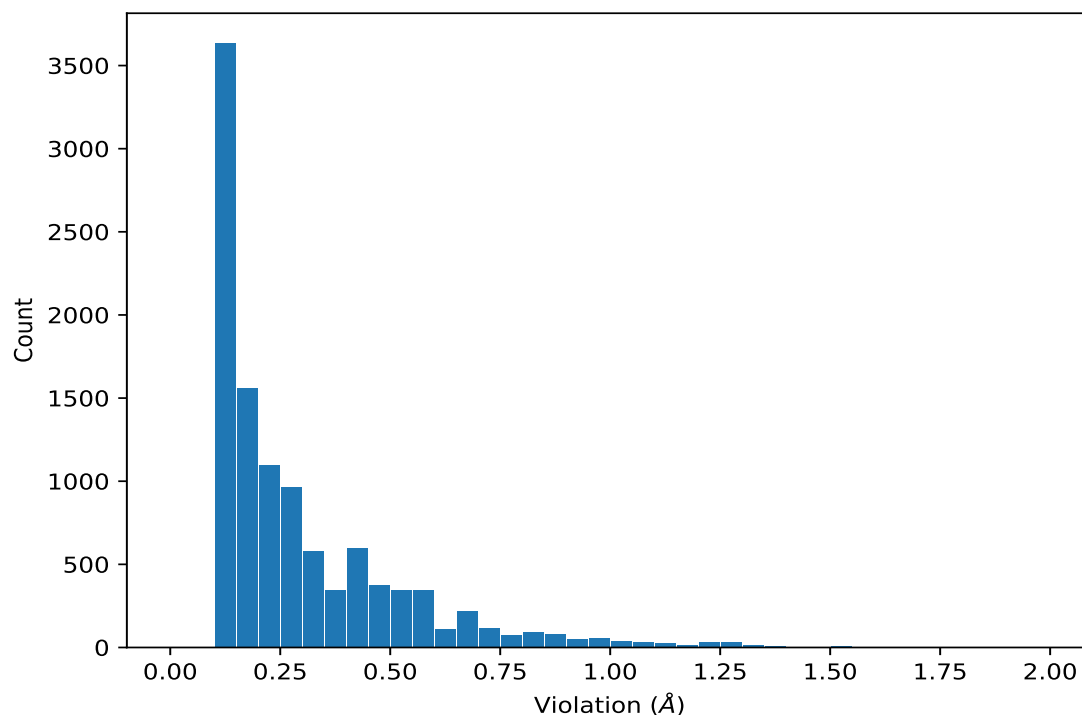
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3471) | 1:76:A:ARG:HA | 1:72:A:GLN:HA | 2 | 0.11 | 0.0 | 0.11 |
| (1,192) | 1:36:A:ARG:HG2 | 1:40:A:SER:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,192) | 1:36:A:ARG:HG3 | 1:40:A:SER:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,2206) | 1:47:A:VAL:HA | 1:59:A:LEU:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2206) | 1:47:A:VAL:HA | 1:59:A:LEU:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD11 | 1:69:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD11 | 1:69:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD12 | 1:69:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD12 | 1:69:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD13 | 1:69:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD13 | 1:69:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD21 | 1:69:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD21 | 1:69:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD22 | 1:69:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD22 | 1:69:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD23 | 1:69:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD23 | 1:69:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,2601) | 1:22:A:ALA:HB1 | 1:96:A:ASN:HA | 2 | 0.11 | 0.0 | 0.11 |
| (1,2601) | 1:22:A:ALA:HB2 | 1:96:A:ASN:HA | 2 | 0.11 | 0.0 | 0.11 |
| (1,2601) | 1:22:A:ALA:HB3 | 1:96:A:ASN:HA | 2 | 0.11 | 0.0 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1030) | 1:65:A:ASN:H | 1:65:A:ASN:HA | 2 | 0.1 | 0.0 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG11 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG12 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG13 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG21 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG22 | 2 | 0.1 | 0.0 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG23 | 2 | 0.1 | 0.0 | 0.1 |
| (1,3135) | 1:170:A:THR:HB | 1:175:A:PRO:HD2 | 2 | 0.1 | 0.0 | 0.1 |
| (1,3135) | 1:170:A:THR:HB | 1:175:A:PRO:HD3 | 2 | 0.1 | 0.0 | 0.1 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB2 | 8 | 1.99 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB3 | 8 | 1.99 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:30:A:THR:HB | 10 | 1.85 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB2 | 20 | 1.68 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB3 | 20 | 1.68 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB2 | 5 | 1.66 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB3 | 5 | 1.66 |
| (1,3793) | 1:48:A:VAL:HG23 | 1:65:A:ASN:HD21 | 12 | 1.64 |
| (1,3793) | 1:48:A:VAL:HG23 | 1:65:A:ASN:HD22 | 12 | 1.64 |
| (1,3553) | 1:87:A:ALA:HB3 | 1:43:A:ILE:HA | 14 | 1.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD21 | 11 | 1.55 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD22 | 11 | 1.55 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB2 | 15 | 1.54 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB3 | 15 | 1.54 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB2 | 16 | 1.54 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB3 | 16 | 1.54 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB2 | 7 | 1.52 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB3 | 7 | 1.52 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB2 | 12 | 1.46 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB3 | 12 | 1.46 |
| (1,3582) | 1:17:A:LEU:HD12 | 1:191:A:PRO:HB2 | 4 | 1.45 |
| (1,3582) | 1:17:A:LEU:HD12 | 1:191:A:PRO:HB3 | 4 | 1.45 |
| (1,3657) | 1:77:A:LEU:HD22 | 1:73:A:ALA:HA | 9 | 1.42 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 5 | 1.41 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 5 | 1.41 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB2 | 11 | 1.37 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB3 | 11 | 1.37 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB2 | 18 | 1.37 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB3 | 18 | 1.37 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:43:A:ILE:HA | 13 | 1.37 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD11 | 13 | 1.35 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD12 | 13 | 1.35 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD13 | 13 | 1.35 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD21 | 13 | 1.35 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD22 | 13 | 1.35 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD23 | 13 | 1.35 |
| (1,3793) | 1:48:A:VAL:HG11 | 1:65:A:ASN:HD21 | 3 | 1.34 |
| (1,3793) | 1:48:A:VAL:HG11 | 1:65:A:ASN:HD22 | 3 | 1.34 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB2 | 5 | 1.32 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB3 | 5 | 1.32 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 3 | 1.31 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 3 | 1.31 |
| (1,2430) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HG | 9 | 1.31 |
| (1,3657) | 1:77:A:LEU:HD12 | 1:73:A:ALA:HA | 3 | 1.3 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 2 | 1.3 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 2 | 1.3 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 2 | 1.3 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 2 | 1.3 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 2 | 1.3 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 2 | 1.3 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB2 | 2 | 1.29 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB3 | 2 | 1.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB2 | 8 | 1.29 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB3 | 8 | 1.29 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB2 | 17 | 1.29 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB3 | 17 | 1.29 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB2 | 14 | 1.28 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB3 | 14 | 1.28 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE1 | 17 | 1.28 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE2 | 17 | 1.28 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA2 | 3 | 1.27 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA3 | 3 | 1.27 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB2 | 9 | 1.26 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB3 | 9 | 1.26 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD11 | 10 | 1.26 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD12 | 10 | 1.26 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD13 | 10 | 1.26 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD21 | 10 | 1.26 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD22 | 10 | 1.26 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD23 | 10 | 1.26 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD11 | 1 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD12 | 1 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD13 | 1 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD21 | 1 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD22 | 1 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD23 | 1 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD11 | 8 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD12 | 8 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD13 | 8 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD21 | 8 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD22 | 8 | 1.25 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD23 | 8 | 1.25 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB1 | 19 | 1.25 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB2 | 19 | 1.25 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB3 | 19 | 1.25 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 18 | 1.24 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 18 | 1.24 |
| (1,3340) | 1:120:A:VAL:HG11 | 1:117:A:LEU:HB2 | 18 | 1.24 |
| (1,3340) | 1:120:A:VAL:HG11 | 1:117:A:LEU:HB3 | 18 | 1.24 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD11 | 9 | 1.24 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD12 | 9 | 1.24 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD13 | 9 | 1.24 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD21 | 9 | 1.24 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD22 | 9 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD23 | 9 | 1.24 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB1 | 10 | 1.22 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB2 | 10 | 1.22 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB3 | 10 | 1.22 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD11 | 14 | 1.22 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD12 | 14 | 1.22 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD13 | 14 | 1.22 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD21 | 14 | 1.22 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD22 | 14 | 1.22 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD23 | 14 | 1.22 |
| (1,3623) | 1:140:A:ILE:HD13 | 1:95:A:PHE:HE1 | 3 | 1.22 |
| (1,3623) | 1:140:A:ILE:HD13 | 1:95:A:PHE:HE2 | 3 | 1.22 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 18 | 1.22 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 18 | 1.22 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB2 | 17 | 1.21 |
| (1,3849) | 1:102:A:ALA:HB1 | 1:104:A:ASN:HB3 | 17 | 1.21 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD21 | 6 | 1.21 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD22 | 6 | 1.21 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB2 | 14 | 1.21 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB3 | 14 | 1.21 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 19 | 1.21 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 19 | 1.21 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:43:A:ILE:HA | 11 | 1.21 |
| (1,3632) | 1:44:A:ALA:HB2 | 1:43:A:ILE:HB | 17 | 1.19 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA2 | 11 | 1.19 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA3 | 11 | 1.19 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB2 | 16 | 1.18 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB3 | 16 | 1.18 |
| (1,3793) | 1:48:A:VAL:HG22 | 1:65:A:ASN:HD21 | 17 | 1.18 |
| (1,3793) | 1:48:A:VAL:HG22 | 1:65:A:ASN:HD22 | 17 | 1.18 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB2 | 11 | 1.18 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB3 | 11 | 1.18 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 10 | 1.18 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 17 | 1.17 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 17 | 1.17 |
| (1,3320) | 1:99:A:VAL:HG13 | 1:100:A:LEU:HB2 | 2 | 1.17 |
| (1,3320) | 1:99:A:VAL:HG13 | 1:100:A:LEU:HB3 | 2 | 1.17 |
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB2 | 9 | 1.15 |
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB3 | 9 | 1.15 |
| (1,3632) | 1:44:A:ALA:HB2 | 1:43:A:ILE:HB | 16 | 1.15 |
| (1,3340) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 15 | 1.15 |
| (1,3340) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 15 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3320) | 1:99:A:VAL:HG12 | 1:100:A:LEU:HB2 | 16 | 1.14 |
| (1,3320) | 1:99:A:VAL:HG12 | 1:100:A:LEU:HB3 | 16 | 1.14 |
| (1,3799) | 1:131:A:VAL:HG22 | 1:51:A:ALA:HA | 16 | 1.13 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA2 | 1 | 1.13 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA3 | 1 | 1.13 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB2 | 7 | 1.12 |
| (1,3849) | 1:102:A:ALA:HB2 | 1:104:A:ASN:HB3 | 7 | 1.12 |
| (1,3340) | 1:120:A:VAL:HG21 | 1:117:A:LEU:HB2 | 14 | 1.12 |
| (1,3340) | 1:120:A:VAL:HG21 | 1:117:A:LEU:HB3 | 14 | 1.12 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:47:A:VAL:HB | 19 | 1.12 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD11 | 5 | 1.12 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD12 | 5 | 1.12 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD13 | 5 | 1.12 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD21 | 5 | 1.12 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD22 | 5 | 1.12 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD23 | 5 | 1.12 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB2 | 10 | 1.11 |
| (1,3582) | 1:17:A:LEU:HD23 | 1:191:A:PRO:HB3 | 10 | 1.11 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD21 | 8 | 1.1 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD22 | 8 | 1.1 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:43:A:ILE:HA | 3 | 1.1 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 6 | 1.1 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 4 | 1.1 |
| (1,3657) | 1:77:A:LEU:HD23 | 1:73:A:ALA:HA | 17 | 1.09 |
| (1,3632) | 1:44:A:ALA:HB3 | 1:48:A:VAL:HB | 12 | 1.09 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:18:A:ILE:HB | 15 | 1.08 |
| (1,3355) | 1:28:A:THR:HG23 | 1:34:A:VAL:HB | 7 | 1.08 |
| (1,3340) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 4 | 1.08 |
| (1,3340) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 4 | 1.08 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:159:A:ALA:HB1 | 4 | 1.07 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:159:A:ALA:HB2 | 4 | 1.07 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:159:A:ALA:HB3 | 4 | 1.07 |
| (1,3632) | 1:44:A:ALA:HB1 | 1:43:A:ILE:HB | 13 | 1.07 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA2 | 12 | 1.07 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA3 | 12 | 1.07 |
| (1,3553) | 1:87:A:ALA:HB3 | 1:43:A:ILE:HA | 12 | 1.07 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:157:A:SER:HB2 | 6 | 1.06 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:157:A:SER:HB3 | 6 | 1.06 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE1 | 11 | 1.06 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE2 | 11 | 1.06 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 15 | 1.06 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD11 | 1 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD12 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD13 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD21 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD22 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD23 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD11 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD12 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD13 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD21 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD22 | 1 | 1.05 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD23 | 1 | 1.05 |
| (1,3657) | 1:77:A:LEU:HD12 | 1:73:A:ALA:HA | 20 | 1.05 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA2 | 4 | 1.05 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA3 | 4 | 1.05 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:50:A:ARG:HG2 | 20 | 1.05 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:50:A:ARG:HG3 | 20 | 1.05 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 18 | 1.04 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 18 | 1.04 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG2 | 2 | 1.04 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG3 | 2 | 1.04 |
| (1,3632) | 1:44:A:ALA:HB1 | 1:48:A:VAL:HB | 3 | 1.03 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB2 | 4 | 1.03 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB3 | 4 | 1.03 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA2 | 8 | 1.02 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA3 | 8 | 1.02 |
| (1,2430) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HG | 8 | 1.02 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 10 | 1.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 10 | 1.01 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 10 | 1.01 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB2 | 8 | 1.01 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB3 | 8 | 1.01 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB1 | 6 | 1.0 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB2 | 6 | 1.0 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB3 | 6 | 1.0 |
| (1,3231) | 1:34:A:VAL:HG22 | 1:139:A:ASP:HA | 11 | 1.0 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 1 | 0.99 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 1 | 0.99 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 1 | 0.99 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 1 | 0.99 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA2 | 9 | 0.99 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA3 | 9 | 0.99 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD2 | 20 | 0.99 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD3 | 20 | 0.99 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 18 | 0.99 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB2 | 1 | 0.98 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB3 | 1 | 0.98 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB2 | 10 | 0.98 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB3 | 10 | 0.98 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HB2 | 11 | 0.98 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HB3 | 11 | 0.98 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD11 | 16 | 0.98 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD12 | 16 | 0.98 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD13 | 16 | 0.98 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD21 | 16 | 0.98 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD22 | 16 | 0.98 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD23 | 16 | 0.98 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 14 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 14 | 0.97 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 14 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 18 | 0.97 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 18 | 0.97 |
| (1,3231) | 1:34:A:VAL:HG13 | 1:36:A:ARG:HA | 5 | 0.97 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD11 | 20 | 0.97 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD12 | 20 | 0.97 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD13 | 20 | 0.97 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD21 | 20 | 0.97 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD22 | 20 | 0.97 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD23 | 20 | 0.97 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB2 | 1 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB3 | 1 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG21 | 1:117:A:LEU:HB2 | 16 | 0.96 |
| (1,3340) | 1:120:A:VAL:HG21 | 1:117:A:LEU:HB3 | 16 | 0.96 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB1 | 16 | 0.96 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB2 | 16 | 0.96 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB3 | 16 | 0.96 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 6 | 0.95 |
| (1,3545) | 1:55:A:LEU:HD13 | 1:49:A:GLN:HB2 | 15 | 0.95 |
| (1,3545) | 1:55:A:LEU:HD13 | 1:49:A:GLN:HB3 | 15 | 0.95 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD11 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD12 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD13 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD21 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD22 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD21 | 1:17:A:LEU:HD23 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD11 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD12 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD13 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD21 | 11 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD22 | 11 | 0.94 |
| (1,3754) | 1:23:A:ASN:HD22 | 1:17:A:LEU:HD23 | 11 | 0.94 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD11 | 4 | 0.94 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD12 | 4 | 0.94 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD13 | 4 | 0.94 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD21 | 4 | 0.94 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD22 | 4 | 0.94 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD23 | 4 | 0.94 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 5 | 0.94 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 5 | 0.94 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 5 | 0.94 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 5 | 0.94 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 5 | 0.94 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 5 | 0.94 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD11 | 12 | 0.93 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD12 | 12 | 0.93 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD13 | 12 | 0.93 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD21 | 12 | 0.93 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD22 | 12 | 0.93 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD23 | 12 | 0.93 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:30:A:THR:HB | 16 | 0.93 |
| (1,3231) | 1:34:A:VAL:HG13 | 1:36:A:ARG:HA | 19 | 0.93 |
| (1,3632) | 1:44:A:ALA:HB2 | 1:43:A:ILE:HB | 6 | 0.92 |
| (1,3799) | 1:131:A:VAL:HG13 | 1:51:A:ALA:HA | 11 | 0.91 |
| (1,3799) | 1:131:A:VAL:HG13 | 1:51:A:ALA:HA | 19 | 0.91 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD11 | 4 | 0.91 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD12 | 4 | 0.91 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD13 | 4 | 0.91 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD21 | 4 | 0.91 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD22 | 4 | 0.91 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD23 | 4 | 0.91 |
| (1,3632) | 1:44:A:ALA:HB2 | 1:48:A:VAL:HB | 4 | 0.91 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 1 | 0.91 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 1 | 0.91 |
| (1,3231) | 1:34:A:VAL:HG13 | 1:36:A:ARG:HA | 14 | 0.91 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA2 | 13 | 0.9 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA3 | 13 | 0.9 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 19 | 0.9 |
| (1,3790) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 8 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 20 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 20 | 0.89 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 20 | 0.89 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA2 | 10 | 0.89 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA3 | 10 | 0.89 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB2 | 6 | 0.89 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB3 | 6 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 7 | 0.89 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 7 | 0.89 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 6 | 0.88 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 6 | 0.88 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 14 | 0.88 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 14 | 0.88 |
| (1,3422) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HB2 | 10 | 0.88 |
| (1,3422) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HB3 | 10 | 0.88 |
| (1,3231) | 1:34:A:VAL:HG12 | 1:36:A:ARG:HA | 9 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 19 | 0.87 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 19 | 0.87 |
| (1,3340) | 1:120:A:VAL:HG23 | 1:117:A:LEU:HB2 | 12 | 0.87 |
| (1,3340) | 1:120:A:VAL:HG23 | 1:117:A:LEU:HB3 | 12 | 0.87 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 19 | 0.86 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 19 | 0.86 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 19 | 0.86 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 19 | 0.86 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 19 | 0.86 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 19 | 0.86 |
| (1,3632) | 1:44:A:ALA:HB3 | 1:43:A:ILE:HB | 8 | 0.86 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB2 | 19 | 0.86 |
| (1,3582) | 1:17:A:LEU:HD13 | 1:191:A:PRO:HB3 | 19 | 0.86 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA2 | 7 | 0.86 |
| (1,3572) | 1:85:A:ALA:HB1 | 1:80:A:GLY:HA3 | 7 | 0.86 |
| (1,3553) | 1:87:A:ALA:HB3 | 1:43:A:ILE:HA | 8 | 0.86 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 10 | 0.86 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:47:A:VAL:HB | 2 | 0.86 |
| (1,3231) | 1:34:A:VAL:HG21 | 1:139:A:ASP:HA | 3 | 0.86 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD11 | 12 | 0.86 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD12 | 12 | 0.86 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD13 | 12 | 0.86 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD21 | 12 | 0.86 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD22 | 12 | 0.86 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD23 | 12 | 0.86 |
| (1,2430) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HG | 13 | 0.86 |
| (1,3906) | 1:136:A:VAL:HG11 | 1:95:A:PHE:HE1 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG11 | 1:95:A:PHE:HE2 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG12 | 1:95:A:PHE:HE1 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG12 | 1:95:A:PHE:HE2 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG13 | 1:95:A:PHE:HE1 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG13 | 1:95:A:PHE:HE2 | 14 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3906) | 1:136:A:VAL:HG21 | 1:95:A:PHE:HE1 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG21 | 1:95:A:PHE:HE2 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG22 | 1:95:A:PHE:HE1 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG22 | 1:95:A:PHE:HE2 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG23 | 1:95:A:PHE:HE1 | 14 | 0.85 |
| (1,3906) | 1:136:A:VAL:HG23 | 1:95:A:PHE:HE2 | 14 | 0.85 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 5 | 0.85 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 5 | 0.85 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 9 | 0.85 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB2 | 7 | 0.85 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB3 | 7 | 0.85 |
| (1,1031) | 1:170:A:THR:HA | 1:169:A:TYR:H | 18 | 0.85 |
| (1,3763) | 1:41:A:GLN:HB3 | 1:45:A:SER:HB2 | 18 | 0.84 |
| (1,3763) | 1:41:A:GLN:HB3 | 1:45:A:SER:HB3 | 18 | 0.84 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB2 | 2 | 0.84 |
| (1,3582) | 1:17:A:LEU:HD21 | 1:191:A:PRO:HB3 | 2 | 0.84 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:105:A:ILE:HD11 | 10 | 0.84 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:105:A:ILE:HD12 | 10 | 0.84 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:105:A:ILE:HD13 | 10 | 0.84 |
| (1,3231) | 1:34:A:VAL:HG23 | 1:139:A:ASP:HA | 18 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD11 | 9 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD12 | 9 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD13 | 9 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD21 | 9 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD22 | 9 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD23 | 9 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD11 | 15 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD12 | 15 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD13 | 15 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD21 | 15 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD22 | 15 | 0.84 |
| (1,3220) | 1:9:A:ALA:HB1 | 1:117:A:LEU:HD23 | 15 | 0.84 |
| (1,3791) | 1:44:A:ALA:HB1 | 1:74:A:VAL:HA | 4 | 0.83 |
| (1,3734) | 1:37:A:THR:HA | 1:136:A:VAL:HB | 10 | 0.83 |
| (1,3734) | 1:37:A:THR:HA | 1:136:A:VAL:HB | 13 | 0.83 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 7 | 0.83 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 7 | 0.83 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 7 | 0.83 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 7 | 0.83 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 7 | 0.83 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 7 | 0.83 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 8 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 8 | 0.83 |
| (1,3231) | 1:34:A:VAL:HG21 | 1:139:A:ASP:HA | 4 | 0.83 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 18 | 0.82 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 18 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 15 | 0.82 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 15 | 0.82 |
| (1,3657) | 1:77:A:LEU:HD21 | 1:73:A:ALA:HA | 14 | 0.82 |
| (1,3623) | 1:140:A:ILE:HD13 | 1:95:A:PHE:HE1 | 19 | 0.82 |
| (1,3623) | 1:140:A:ILE:HD13 | 1:95:A:PHE:HE2 | 19 | 0.82 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 11 | 0.82 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 11 | 0.82 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:43:A:ILE:HA | 20 | 0.82 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD11 | 3 | 0.82 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD12 | 3 | 0.82 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD13 | 3 | 0.82 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD21 | 3 | 0.82 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD22 | 3 | 0.82 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD23 | 3 | 0.82 |
| (1,2430) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HG | 12 | 0.82 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 17 | 0.81 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 17 | 0.81 |
| (1,3415) | 1:41:A:GLN:HA | 1:42:A:GLN:HA | 17 | 0.81 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD2 | 14 | 0.81 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD3 | 14 | 0.81 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 6 | 0.81 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD2 | 16 | 0.81 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD3 | 16 | 0.81 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG2 | 1 | 0.8 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG3 | 1 | 0.8 |
| (1,3553) | 1:87:A:ALA:HB3 | 1:43:A:ILE:HA | 17 | 0.8 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 10 | 0.8 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 10 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB1 | 12 | 0.8 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB2 | 12 | 0.8 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB3 | 12 | 0.8 |
| (1,3231) | 1:34:A:VAL:HG22 | 1:139:A:ASP:HA | 1 | 0.8 |
| (1,3231) | 1:34:A:VAL:HG23 | 1:139:A:ASP:HA | 2 | 0.8 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 2 | 0.79 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 2 | 0.79 |
| (1,3340) | 1:120:A:VAL:HG11 | 1:117:A:LEU:HB2 | 3 | 0.79 |
| (1,3340) | 1:120:A:VAL:HG11 | 1:117:A:LEU:HB3 | 3 | 0.79 |
| (1,3632) | 1:44:A:ALA:HB1 | 1:48:A:VAL:HB | 11 | 0.78 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 9 | 0.78 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 9 | 0.78 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 14 | 0.78 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 14 | 0.78 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 14 | 0.78 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 14 | 0.78 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 14 | 0.78 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 14 | 0.78 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB2 | 17 | 0.78 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB3 | 17 | 0.78 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB2 | 6 | 0.78 |
| (1,3340) | 1:120:A:VAL:HG12 | 1:117:A:LEU:HB3 | 6 | 0.78 |
| (1,3799) | 1:131:A:VAL:HG11 | 1:51:A:ALA:HA | 12 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 8 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 8 | 0.77 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 8 | 0.77 |
| (1,3657) | 1:77:A:LEU:HD12 | 1:73:A:ALA:HA | 8 | 0.77 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 1 | 0.77 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 1 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 10 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 10 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:47:A:VAL:HB | 14 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 18 | 0.77 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 18 | 0.77 |
| (1,3213) | 1:129:A:ILE:HD13 | 1:50:A:ARG:HG2 | 20 | 0.77 |
| (1,3213) | 1:129:A:ILE:HD13 | 1:50:A:ARG:HG3 | 20 | 0.77 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 19 | 0.77 |
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 7 | 0.77 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 7 | 0.76 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 7 | 0.76 |
| (1,3340) | 1:120:A:VAL:HG23 | 1:117:A:LEU:HB2 | 19 | 0.76 |
| (1,3340) | 1:120:A:VAL:HG23 | 1:117:A:LEU:HB3 | 19 | 0.76 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB1 | 19 | 0.75 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB2 | 19 | 0.75 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB3 | 19 | 0.75 |
| (1,3735) | 1:48:A:VAL:HG23 | 1:46:A:SER:H | 5 | 0.75 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 2 | 0.75 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 2 | 0.75 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 5 | 0.75 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 5 | 0.75 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB2 | 20 | 0.75 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB3 | 20 | 0.75 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB2 | 9 | 0.75 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB3 | 9 | 0.75 |
| (1,3292) | 1:13:A:ALA:H | 1:108:A:LEU:HG | 2 | 0.75 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 9 | 0.75 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 9 | 0.75 |
| (1,1169) | 1:42:A:GLN:HE21 | 1:42:A:GLN:HA | 4 | 0.75 |
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG12 | 1 | 0.75 |
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG13 | 1 | 0.75 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB1 | 8 | 0.75 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB2 | 8 | 0.75 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB3 | 8 | 0.75 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 11 | 0.74 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 11 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 11 | 0.74 |
| (1,3735) | 1:48:A:VAL:HG22 | 1:46:A:SER:H | 7 | 0.74 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD11 | 8 | 0.74 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD12 | 8 | 0.74 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD13 | 8 | 0.74 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD21 | 8 | 0.74 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD22 | 8 | 0.74 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD23 | 8 | 0.74 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 9 | 0.74 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 9 | 0.74 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 2 | 0.74 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 2 | 0.74 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 4 | 0.74 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 4 | 0.74 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 7 | 0.74 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 7 | 0.74 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 2 | 0.74 |
| (1,3231) | 1:34:A:VAL:HG13 | 1:36:A:ARG:HA | 6 | 0.74 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 4 | 0.74 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 4 | 0.74 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 19 | 0.74 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 19 | 0.74 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB1 | 9 | 0.73 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB2 | 9 | 0.73 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB3 | 9 | 0.73 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 2 | 0.73 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 2 | 0.73 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 2 | 0.73 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 4 | 0.73 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 4 | 0.73 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 4 | 0.73 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 20 | 0.73 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 20 | 0.73 |
| (1,3231) | 1:34:A:VAL:HG13 | 1:36:A:ARG:HA | 12 | 0.73 |
| (1,1976) | 1:32:A:ARG:HG2 | 1:33:A:THR:HA | 8 | 0.73 |
| (1,1976) | 1:32:A:ARG:HG3 | 1:33:A:THR:HA | 8 | 0.73 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 9 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 9 | 0.72 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 9 | 0.72 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 16 | 0.72 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 16 | 0.72 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 16 | 0.72 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 12 | 0.72 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 12 | 0.72 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB2 | 14 | 0.72 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB3 | 14 | 0.72 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 1 | 0.72 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 1 | 0.72 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 1 | 0.72 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 1 | 0.72 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 1 | 0.72 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 1 | 0.72 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB2 | 12 | 0.72 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB3 | 12 | 0.72 |
| (1,3553) | 1:87:A:ALA:HB3 | 1:43:A:ILE:HA | 18 | 0.72 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 6 | 0.72 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 6 | 0.72 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB2 | 20 | 0.72 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB3 | 20 | 0.72 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 14 | 0.72 |
| (1,3292) | 1:13:A:ALA:H | 1:108:A:LEU:HG | 10 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 15 | 0.72 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 15 | 0.72 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 16 | 0.72 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 16 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 16 | 0.72 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 16 | 0.72 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 16 | 0.72 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 16 | 0.72 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB1 | 15 | 0.71 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB2 | 15 | 0.71 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB3 | 15 | 0.71 |
| (1,3793) | 1:48:A:VAL:HG13 | 1:65:A:ASN:HD21 | 4 | 0.71 |
| (1,3793) | 1:48:A:VAL:HG13 | 1:65:A:ASN:HD22 | 4 | 0.71 |
| (1,3790) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HA | 7 | 0.71 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 20 | 0.71 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 2 | 0.71 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 2 | 0.71 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB2 | 20 | 0.71 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB3 | 20 | 0.71 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG21 | 19 | 0.71 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG22 | 19 | 0.71 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG23 | 19 | 0.71 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 9 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD11 | 5 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD12 | 5 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD13 | 5 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG11 | 19 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG12 | 19 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG13 | 19 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG21 | 19 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG22 | 19 | 0.71 |
| (1,3344) | 1:93:A:ALA:HB3 | 1:21:A:VAL:HG23 | 19 | 0.71 |
| (1,3231) | 1:34:A:VAL:HG12 | 1:36:A:ARG:HA | 13 | 0.71 |
| (1,1803) | 1:177:A:THR:H | 1:179:A:PRO:HA | 12 | 0.71 |
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB2 | 12 | 0.7 |
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB3 | 12 | 0.7 |
| (1,3818) | 1:87:A:ALA:HB1 | 1:86:A:TYR:HA | 10 | 0.7 |
| (1,3657) | 1:77:A:LEU:HD23 | 1:73:A:ALA:HA | 1 | 0.7 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB2 | 19 | 0.7 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB3 | 19 | 0.7 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 1 | 0.7 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 1 | 0.7 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:43:A:ILE:HA | 4 | 0.7 |
| (1,3409) | 1:88:A:GLN:HB2 | 1:84:A:SER:HA | 10 | 0.7 |
| (1,1095) | 1:193:A:GLY:H | 1:194:A:GLN:HA | 13 | 0.7 |
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE21 | 17 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE22 | 17 | 0.7 |
| (1,1031) | 1:170:A:THR:HA | 1:169:A:TYR:H | 4 | 0.7 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 17 | 0.69 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 17 | 0.69 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:46:A:SER:HB2 | 10 | 0.69 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:46:A:SER:HB3 | 10 | 0.69 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 13 | 0.69 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 13 | 0.69 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 13 | 0.69 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG21 | 4 | 0.69 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG22 | 4 | 0.69 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG23 | 4 | 0.69 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG21 | 16 | 0.69 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG22 | 16 | 0.69 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG23 | 16 | 0.69 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 13 | 0.69 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 13 | 0.69 |
| (1,3292) | 1:112:A:VAL:H | 1:108:A:LEU:HG | 4 | 0.69 |
| (1,3231) | 1:34:A:VAL:HG23 | 1:139:A:ASP:HA | 16 | 0.69 |
| (1,1143) | 1:127:A:LEU:H | 1:124:A:ALA:HB1 | 19 | 0.69 |
| (1,1143) | 1:127:A:LEU:H | 1:124:A:ALA:HB2 | 19 | 0.69 |
| (1,1143) | 1:127:A:LEU:H | 1:124:A:ALA:HB3 | 19 | 0.69 |
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE21 | 20 | 0.69 |
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE22 | 20 | 0.69 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 4 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 4 | 0.68 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 4 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD11 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD12 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD13 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD21 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD22 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE1 | 1:17:A:LEU:HD23 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD11 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD12 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD13 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD21 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD22 | 7 | 0.68 |
| (1,3754) | 1:90:A:PHE:HE2 | 1:17:A:LEU:HD23 | 7 | 0.68 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 17 | 0.68 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 17 | 0.68 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 17 | 0.68 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 4 | 0.68 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 4 | 0.68 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE1 | 10 | 0.68 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE2 | 10 | 0.68 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG21 | 13 | 0.68 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG22 | 13 | 0.68 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG23 | 13 | 0.68 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 5 | 0.68 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 5 | 0.68 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 3 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 3 | 0.68 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 3 | 0.68 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 4 | 0.68 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 8 | 0.68 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB1 | 10 | 0.68 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB2 | 10 | 0.68 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB3 | 10 | 0.68 |
| (1,3790) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 19 | 0.67 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG2 | 13 | 0.67 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG3 | 13 | 0.67 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 15 | 0.67 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 15 | 0.67 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 15 | 0.67 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 2 | 0.67 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB1 | 3 | 0.67 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB2 | 3 | 0.67 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB3 | 3 | 0.67 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HG21 | 12 | 0.67 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HG22 | 12 | 0.67 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:43:A:ILE:HG23 | 12 | 0.67 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG21 | 18 | 0.67 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG22 | 18 | 0.67 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG23 | 18 | 0.67 |
| (1,3464) | 1:126:A:GLY:HA2 | 1:125:A:GLN:HA | 10 | 0.67 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HB2 | 14 | 0.67 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HB3 | 14 | 0.67 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB2 | 17 | 0.67 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB3 | 17 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB1 | 4 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB2 | 4 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB3 | 4 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB1 | 9 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB2 | 9 | 0.67 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB3 | 9 | 0.67 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 5 | 0.66 |
| (1,3735) | 1:48:A:VAL:HG21 | 1:46:A:SER:H | 20 | 0.66 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 20 | 0.66 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 20 | 0.66 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA2 | 7 | 0.66 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA3 | 7 | 0.66 |
| (1,3657) | 1:77:A:LEU:HD22 | 1:73:A:ALA:HA | 5 | 0.66 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 20 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 20 | 0.66 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB1 | 11 | 0.66 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB2 | 11 | 0.66 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB3 | 11 | 0.66 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG21 | 14 | 0.66 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG22 | 14 | 0.66 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG23 | 14 | 0.66 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:132:A:ASP:HB2 | 4 | 0.66 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:132:A:ASP:HB3 | 4 | 0.66 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB2 | 5 | 0.66 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB3 | 5 | 0.66 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 19 | 0.66 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 19 | 0.66 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 19 | 0.66 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 19 | 0.66 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 19 | 0.66 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 19 | 0.66 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 10 | 0.65 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 10 | 0.65 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB2 | 2 | 0.65 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB3 | 2 | 0.65 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 16 | 0.65 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 16 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD11 | 11 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD12 | 11 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD13 | 11 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD21 | 11 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD22 | 11 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD23 | 11 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 17 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 17 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 17 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 17 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 17 | 0.65 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 17 | 0.65 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 9 | 0.65 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 9 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 14 | 0.65 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 14 | 0.65 |
| (1,3464) | 1:126:A:GLY:HA2 | 1:125:A:GLN:HA | 4 | 0.65 |
| (1,3464) | 1:134:A:GLY:HA2 | 1:133:A:SER:HA | 16 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 18 | 0.65 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 18 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 20 | 0.65 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 20 | 0.65 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB1 | 7 | 0.65 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB2 | 7 | 0.65 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB3 | 7 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB1 | 3 | 0.64 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB2 | 3 | 0.64 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB3 | 3 | 0.64 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 5 | 0.64 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 5 | 0.64 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 5 | 0.64 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 7 | 0.64 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 7 | 0.64 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 7 | 0.64 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA2 | 9 | 0.64 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA3 | 9 | 0.64 |
| (1,2430) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HG | 5 | 0.64 |
| (1,1095) | 1:193:A:GLY:H | 1:194:A:GLN:HA | 7 | 0.64 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 7 | 0.63 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 7 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 3 | 0.63 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 3 | 0.63 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 19 | 0.63 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 19 | 0.63 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 19 | 0.63 |
| (1,3660) | 1:172:A:PRO:HG2 | 1:18:A:ILE:HG12 | 3 | 0.63 |
| (1,3660) | 1:172:A:PRO:HG2 | 1:18:A:ILE:HG13 | 3 | 0.63 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE1 | 2 | 0.63 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE2 | 2 | 0.63 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 2 | 0.63 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 2 | 0.63 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 6 | 0.63 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 6 | 0.63 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB2 | 19 | 0.63 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB3 | 19 | 0.63 |
| (1,3319) | 1:61:A:VAL:HG22 | 1:65:A:ASN:HB2 | 9 | 0.63 |
| (1,3319) | 1:61:A:VAL:HG22 | 1:65:A:ASN:HB3 | 9 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD11 | 10 | 0.63 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD12 | 10 | 0.63 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD13 | 10 | 0.63 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD21 | 10 | 0.63 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD22 | 10 | 0.63 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD23 | 10 | 0.63 |
| (1,3213) | 1:129:A:ILE:HD12 | 1:50:A:ARG:HG2 | 14 | 0.63 |
| (1,3213) | 1:129:A:ILE:HD12 | 1:50:A:ARG:HG3 | 14 | 0.63 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 1 | 0.62 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 1 | 0.62 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 1 | 0.62 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:135:A:SER:HB2 | 17 | 0.62 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:135:A:SER:HB3 | 17 | 0.62 |
| (1,3734) | 1:131:A:VAL:HA | 1:136:A:VAL:HB | 5 | 0.62 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 20 | 0.62 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 20 | 0.62 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 15 | 0.62 |
| (1,3655) | 1:87:A:ALA:HB3 | 1:35:A:LEU:HA | 19 | 0.62 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 18 | 0.62 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 18 | 0.62 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 18 | 0.62 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 18 | 0.62 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 18 | 0.62 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 18 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG21 | 9 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG22 | 9 | 0.62 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:43:A:ILE:HG23 | 9 | 0.62 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 11 | 0.62 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 11 | 0.62 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB1 | 17 | 0.62 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB2 | 17 | 0.62 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB3 | 17 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 9 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 9 | 0.62 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 9 | 0.62 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD11 | 13 | 0.62 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD12 | 13 | 0.62 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD13 | 13 | 0.62 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD21 | 13 | 0.62 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD22 | 13 | 0.62 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD23 | 13 | 0.62 |
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 5 | 0.62 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 4 | 0.61 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 4 | 0.61 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 4 | 0.61 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB2 | 2 | 0.61 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB3 | 2 | 0.61 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB2 | 20 | 0.61 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB3 | 20 | 0.61 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB1 | 5 | 0.61 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB2 | 5 | 0.61 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB3 | 5 | 0.61 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 14 | 0.61 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 14 | 0.61 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB2 | 5 | 0.61 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB3 | 5 | 0.61 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB2 | 13 | 0.61 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB3 | 13 | 0.61 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA2 | 11 | 0.61 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA3 | 11 | 0.61 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 9 | 0.61 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB2 | 15 | 0.6 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB3 | 15 | 0.6 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB1 | 12 | 0.6 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB2 | 12 | 0.6 |
| (1,3811) | 1:70:A:ALA:HB3 | 1:51:A:ALA:HB3 | 12 | 0.6 |
| (1,3790) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 3 | 0.6 |
| (1,3758) | 1:120:A:VAL:HG23 | 1:124:A:ALA:HB1 | 13 | 0.6 |
| (1,3758) | 1:120:A:VAL:HG23 | 1:124:A:ALA:HB2 | 13 | 0.6 |
| (1,3758) | 1:120:A:VAL:HG23 | 1:124:A:ALA:HB3 | 13 | 0.6 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 12 | 0.6 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 12 | 0.6 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 12 | 0.6 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 6 | 0.6 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 6 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3582) | 1:17:A:LEU:HD12 | 1:191:A:PRO:HB2 | 3 | 0.6 |
| (1,3582) | 1:17:A:LEU:HD12 | 1:191:A:PRO:HB3 | 3 | 0.6 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB1 | 20 | 0.6 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB2 | 20 | 0.6 |
| (1,3580) | 1:101:A:ASN:HB3 | 1:102:A:ALA:HB3 | 20 | 0.6 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 17 | 0.6 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 17 | 0.6 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD2 | 9 | 0.6 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD3 | 9 | 0.6 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB1 | 10 | 0.6 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB2 | 10 | 0.6 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB3 | 10 | 0.6 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 1 | 0.6 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 15 | 0.6 |
| (1,3319) | 1:61:A:VAL:HG23 | 1:65:A:ASN:HB2 | 14 | 0.6 |
| (1,3319) | 1:61:A:VAL:HG23 | 1:65:A:ASN:HB3 | 14 | 0.6 |
| (1,3292) | 1:13:A:ALA:H | 1:108:A:LEU:HG | 18 | 0.6 |
| (1,1145) | 1:127:A:LEU:H | 1:129:A:ILE:HG21 | 13 | 0.6 |
| (1,1145) | 1:127:A:LEU:H | 1:129:A:ILE:HG22 | 13 | 0.6 |
| (1,1145) | 1:127:A:LEU:H | 1:129:A:ILE:HG23 | 13 | 0.6 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD11 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD12 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD13 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD21 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD22 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD23 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD11 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD12 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD13 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD21 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD22 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD23 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD11 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD12 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD13 | 8 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD21 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD22 | 8 | 0.59 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD23 | 8 | 0.59 |
| (1,3849) | 1:51:A:ALA:HB3 | 1:132:A:ASP:HB2 | 6 | 0.59 |
| (1,3849) | 1:51:A:ALA:HB3 | 1:132:A:ASP:HB3 | 6 | 0.59 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 5 | 0.59 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 5 | 0.59 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 6 | 0.59 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 6 | 0.59 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 6 | 0.59 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD11 | 4 | 0.59 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD12 | 4 | 0.59 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD13 | 4 | 0.59 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD21 | 4 | 0.59 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD22 | 4 | 0.59 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD23 | 4 | 0.59 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB2 | 16 | 0.59 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB3 | 16 | 0.59 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE1 | 4 | 0.59 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE2 | 4 | 0.59 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB2 | 2 | 0.59 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB3 | 2 | 0.59 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 20 | 0.59 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 12 | 0.59 |
| (1,3344) | 1:93:A:ALA:HB1 | 1:105:A:ILE:HD11 | 16 | 0.59 |
| (1,3344) | 1:93:A:ALA:HB1 | 1:105:A:ILE:HD12 | 16 | 0.59 |
| (1,3344) | 1:93:A:ALA:HB1 | 1:105:A:ILE:HD13 | 16 | 0.59 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 3 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB1 | 1 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB2 | 1 | 0.58 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB3 | 1 | 0.58 |
| (1,3785) | 1:3:A:PRO:HB3 | 1:9:A:ALA:HB1 | 18 | 0.58 |
| (1,3785) | 1:3:A:PRO:HB3 | 1:9:A:ALA:HB2 | 18 | 0.58 |
| (1,3785) | 1:3:A:PRO:HB3 | 1:9:A:ALA:HB3 | 18 | 0.58 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 9 | 0.58 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 9 | 0.58 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 9 | 0.58 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:14:A:SER:HB2 | 10 | 0.58 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:14:A:SER:HB3 | 10 | 0.58 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD11 | 15 | 0.58 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD12 | 15 | 0.58 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD13 | 15 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD21 | 15 | 0.58 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD22 | 15 | 0.58 |
| (1,3644) | 1:113:A:LEU:HD13 | 1:17:A:LEU:HD23 | 15 | 0.58 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 15 | 0.58 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 15 | 0.58 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 5 | 0.58 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 5 | 0.58 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 5 | 0.58 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 5 | 0.58 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 5 | 0.58 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 5 | 0.58 |
| (1,3460) | 1:85:A:ALA:HB3 | 1:84:A:SER:HA | 10 | 0.58 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 18 | 0.58 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 18 | 0.58 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD2 | 19 | 0.58 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD3 | 19 | 0.58 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD2 | 19 | 0.58 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD3 | 19 | 0.58 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB1 | 13 | 0.58 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB2 | 13 | 0.58 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB3 | 13 | 0.58 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD11 | 6 | 0.58 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD12 | 6 | 0.58 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD13 | 6 | 0.58 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD21 | 6 | 0.58 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD22 | 6 | 0.58 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD23 | 6 | 0.58 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 4 | 0.58 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 4 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 1 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 1 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 1 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 1 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 1 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 1 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 5 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 5 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 5 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 5 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 5 | 0.58 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 5 | 0.58 |
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG12 | 14 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG13 | 14 | 0.58 |
| (1,1065) | 1:50:A:ARG:HB2 | 1:50:A:ARG:HE | 20 | 0.58 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 10 | 0.58 |
| (1,989) | 1:110:A:SER:H | 1:117:A:LEU:HG | 16 | 0.58 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 20 | 0.58 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 20 | 0.57 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB2 | 16 | 0.57 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB3 | 16 | 0.57 |
| (1,3692) | 1:117:A:LEU:HG | 1:105:A:ILE:HG21 | 10 | 0.57 |
| (1,3692) | 1:117:A:LEU:HG | 1:105:A:ILE:HG22 | 10 | 0.57 |
| (1,3692) | 1:117:A:LEU:HG | 1:105:A:ILE:HG23 | 10 | 0.57 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA2 | 11 | 0.57 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA3 | 11 | 0.57 |
| (1,3654) | 1:39:A:VAL:HG13 | 1:38:A:GLY:HA2 | 9 | 0.57 |
| (1,3654) | 1:39:A:VAL:HG13 | 1:38:A:GLY:HA3 | 9 | 0.57 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 7 | 0.57 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 7 | 0.57 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD11 | 6 | 0.57 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD12 | 6 | 0.57 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD13 | 6 | 0.57 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD21 | 6 | 0.57 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD22 | 6 | 0.57 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD23 | 6 | 0.57 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB2 | 18 | 0.57 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB3 | 18 | 0.57 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 13 | 0.57 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB2 | 5 | 0.57 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB3 | 5 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG2 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG3 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG2 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG3 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG2 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG3 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG2 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG3 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG2 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG3 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG2 | 17 | 0.57 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG3 | 17 | 0.57 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 7 | 0.57 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 7 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 7 | 0.57 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 7 | 0.57 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 7 | 0.57 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 7 | 0.57 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 7 | 0.57 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 7 | 0.57 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 7 | 0.57 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 5 | 0.57 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB1 | 6 | 0.57 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB2 | 6 | 0.57 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB3 | 6 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG11 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG12 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG13 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG21 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG22 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG23 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG11 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG12 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG13 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG21 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG22 | 9 | 0.57 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG23 | 9 | 0.57 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 12 | 0.57 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 12 | 0.57 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 12 | 0.57 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 12 | 0.57 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 12 | 0.57 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 12 | 0.57 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB2 | 2 | 0.57 |
| (1,3340) | 1:120:A:VAL:HG13 | 1:117:A:LEU:HB3 | 2 | 0.57 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB1 | 2 | 0.57 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB2 | 2 | 0.57 |
| (1,3251) | 1:136:A:VAL:HB | 1:51:A:ALA:HB3 | 2 | 0.57 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 3 | 0.57 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 3 | 0.57 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 18 | 0.57 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 18 | 0.57 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 18 | 0.57 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 18 | 0.57 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 18 | 0.57 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 18 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB1 | 9 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB2 | 9 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB3 | 9 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 13 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 13 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 13 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 13 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 13 | 0.57 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 13 | 0.57 |
| (1,3910) | 1:39:A:VAL:HA | 1:86:A:TYR:HD1 | 20 | 0.56 |
| (1,3910) | 1:39:A:VAL:HA | 1:86:A:TYR:HD2 | 20 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD11 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD12 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD13 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD21 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD22 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD23 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD11 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD12 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD13 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD21 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD22 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD23 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD11 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD12 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD13 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD21 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD22 | 19 | 0.56 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD23 | 19 | 0.56 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB2 | 18 | 0.56 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB3 | 18 | 0.56 |
| (1,3799) | 1:131:A:VAL:HG13 | 1:51:A:ALA:HA | 9 | 0.56 |
| (1,3791) | 1:44:A:ALA:HB2 | 1:74:A:VAL:HA | 5 | 0.56 |
| (1,3768) | 1:172:A:PRO:HG2 | 1:24:A:ALA:HB1 | 3 | 0.56 |
| (1,3768) | 1:172:A:PRO:HG2 | 1:24:A:ALA:HB2 | 3 | 0.56 |
| (1,3768) | 1:172:A:PRO:HG2 | 1:24:A:ALA:HB3 | 3 | 0.56 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 3 | 0.56 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 3 | 0.56 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 3 | 0.56 |
| (1,3683) | 1:51:A:ALA:HB1 | 1:50:A:ARG:HA | 7 | 0.56 |
| (1,3683) | 1:51:A:ALA:HB2 | 1:50:A:ARG:HA | 10 | 0.56 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB1 | 4 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB2 | 4 | 0.56 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB3 | 4 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG21 | 3 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG22 | 3 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:43:A:ILE:HG23 | 3 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD11 | 15 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD12 | 15 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD13 | 15 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD21 | 15 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD22 | 15 | 0.56 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD23 | 15 | 0.56 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 3 | 0.56 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 3 | 0.56 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 7 | 0.56 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 7 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD11 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD12 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD13 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD11 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD12 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD13 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD11 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD12 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD13 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD11 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD12 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD13 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD11 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD12 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD13 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD11 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD12 | 9 | 0.56 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD13 | 9 | 0.56 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD2 | 3 | 0.56 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD3 | 3 | 0.56 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB2 | 8 | 0.56 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB3 | 8 | 0.56 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD11 | 13 | 0.56 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD12 | 13 | 0.56 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD13 | 13 | 0.56 |
| (1,3309) | 1:85:A:ALA:HA | 1:86:A:TYR:HB2 | 10 | 0.56 |
| (1,3309) | 1:85:A:ALA:HA | 1:86:A:TYR:HB3 | 10 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 20 | 0.56 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 17 | 0.56 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 20 | 0.56 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 20 | 0.56 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD2 | 6 | 0.56 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD3 | 6 | 0.56 |
| (1,3799) | 1:131:A:VAL:HG11 | 1:51:A:ALA:HA | 4 | 0.55 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 10 | 0.55 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 9 | 0.55 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB2 | 15 | 0.55 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB3 | 15 | 0.55 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA2 | 6 | 0.55 |
| (1,3572) | 1:85:A:ALA:HB2 | 1:80:A:GLY:HA3 | 6 | 0.55 |
| (1,3513) | 1:85:A:ALA:HB2 | 1:81:A:SER:HB2 | 8 | 0.55 |
| (1,3513) | 1:85:A:ALA:HB2 | 1:81:A:SER:HB3 | 8 | 0.55 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 17 | 0.55 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 17 | 0.55 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 16 | 0.55 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 2 | 0.55 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD11 | 1 | 0.55 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD12 | 1 | 0.55 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD13 | 1 | 0.55 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD11 | 18 | 0.55 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD12 | 18 | 0.55 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD13 | 18 | 0.55 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD21 | 18 | 0.55 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD22 | 18 | 0.55 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD23 | 18 | 0.55 |
| (1,3173) | 1:177:A:THR:HG21 | 1:190:A:ALA:HA | 17 | 0.55 |
| (1,3173) | 1:177:A:THR:HG22 | 1:190:A:ALA:HA | 17 | 0.55 |
| (1,3173) | 1:177:A:THR:HG23 | 1:190:A:ALA:HA | 17 | 0.55 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 17 | 0.55 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 17 | 0.55 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 17 | 0.55 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 17 | 0.55 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 17 | 0.55 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 17 | 0.55 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB1 | 13 | 0.54 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB2 | 13 | 0.54 |
| (1,3811) | 1:70:A:ALA:HB2 | 1:51:A:ALA:HB3 | 13 | 0.54 |
| (1,3799) | 1:131:A:VAL:HG13 | 1:51:A:ALA:HA | 18 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 12 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 12 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 17 | 0.54 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 17 | 0.54 |
| (1,3561) | 1:111:A:ARG:HD3 | 1:111:A:ARG:HA | 9 | 0.54 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 2 | 0.54 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 2 | 0.54 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 5 | 0.54 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 19 | 0.54 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB2 | 18 | 0.54 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB3 | 18 | 0.54 |
| (1,3286) | 1:48:A:VAL:HG21 | 1:47:A:VAL:HB | 15 | 0.54 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD11 | 5 | 0.54 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD12 | 5 | 0.54 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD13 | 5 | 0.54 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD21 | 5 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD22 | 5 | 0.54 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD23 | 5 | 0.54 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 20 | 0.54 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 20 | 0.54 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 20 | 0.54 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 20 | 0.54 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 20 | 0.54 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 20 | 0.54 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 10 | 0.54 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 10 | 0.54 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 10 | 0.54 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 10 | 0.54 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 10 | 0.54 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 10 | 0.54 |
| (1,1017) | 1:102:A:ALA:H | 1:105:A:ILE:HD11 | 14 | 0.54 |
| (1,1017) | 1:102:A:ALA:H | 1:105:A:ILE:HD12 | 14 | 0.54 |
| (1,1017) | 1:102:A:ALA:H | 1:105:A:ILE:HD13 | 14 | 0.54 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 6 | 0.53 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB1 | 19 | 0.53 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB2 | 19 | 0.53 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB3 | 19 | 0.53 |
| (1,3756) | 1:156:A:TYR:HB2 | 1:157:A:SER:HA | 20 | 0.53 |
| (1,3683) | 1:51:A:ALA:HB3 | 1:50:A:ARG:HA | 8 | 0.53 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 13 | 0.53 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 13 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 13 | 0.53 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 13 | 0.53 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD11 | 11 | 0.53 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD12 | 11 | 0.53 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD13 | 11 | 0.53 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD21 | 11 | 0.53 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD22 | 11 | 0.53 |
| (1,3579) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HD23 | 11 | 0.53 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB2 | 8 | 0.53 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB3 | 8 | 0.53 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 7 | 0.53 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 7 | 0.53 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 7 | 0.53 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 7 | 0.53 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 7 | 0.53 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 7 | 0.53 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 10 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 10 | 0.53 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 12 | 0.53 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 12 | 0.53 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG2 | 5 | 0.53 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG3 | 5 | 0.53 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 6 | 0.53 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 20 | 0.53 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 20 | 0.53 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 20 | 0.53 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 10 | 0.53 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB2 | 17 | 0.53 |
| (1,3340) | 1:120:A:VAL:HG22 | 1:117:A:LEU:HB3 | 17 | 0.53 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD11 | 12 | 0.53 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD12 | 12 | 0.53 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD13 | 12 | 0.53 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD21 | 12 | 0.53 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD22 | 12 | 0.53 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD23 | 12 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 3 | 0.53 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 3 | 0.53 |
| (1,1814) | 1:104:A:ASN:HD22 | 1:108:A:LEU:HG | 15 | 0.53 |
| (1,1095) | 1:193:A:GLY:H | 1:191:A:PRO:HA | 6 | 0.53 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG11 | 15 | 0.53 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG12 | 15 | 0.53 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG13 | 15 | 0.53 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG21 | 15 | 0.53 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG22 | 15 | 0.53 |
| (1,1034) | 1:109:A:GLY:H | 1:112:A:VAL:HG23 | 15 | 0.53 |
| (1,1031) | 1:170:A:THR:HA | 1:169:A:TYR:H | 11 | 0.53 |
| (1,3748) | 1:50:A:ARG:HD2 | 1:55:A:LEU:HA | 10 | 0.52 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 1 | 0.52 |
| (1,3695) | 1:150:A:SER:HB3 | 1:147:A:LEU:HA | 2 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3683) | 1:56:A:ALA:HB1 | 1:50:A:ARG:HA | 1 | 0.52 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA2 | 14 | 0.52 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA3 | 14 | 0.52 |
| (1,3657) | 1:77:A:LEU:HD21 | 1:73:A:ALA:HA | 6 | 0.52 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB2 | 10 | 0.52 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB3 | 10 | 0.52 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE21 | 14 | 0.52 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE22 | 14 | 0.52 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB2 | 9 | 0.52 |
| (1,3582) | 1:17:A:LEU:HD22 | 1:191:A:PRO:HB3 | 9 | 0.52 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB2 | 3 | 0.52 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB3 | 3 | 0.52 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 15 | 0.52 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 15 | 0.52 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD11 | 19 | 0.52 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD12 | 19 | 0.52 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD13 | 19 | 0.52 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD21 | 19 | 0.52 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD22 | 19 | 0.52 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD23 | 19 | 0.52 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 2 | 0.52 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 2 | 0.52 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 8 | 0.52 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 8 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG2 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG3 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG2 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG3 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG2 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG3 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG2 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG3 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG2 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG3 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG2 | 11 | 0.52 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG3 | 11 | 0.52 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 14 | 0.52 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 3 | 0.52 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 11 | 0.52 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD11 | 7 | 0.52 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD12 | 7 | 0.52 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD13 | 7 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD21 | 7 | 0.52 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD22 | 7 | 0.52 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD23 | 7 | 0.52 |
| (1,3319) | 1:61:A:VAL:HG11 | 1:65:A:ASN:HB2 | 2 | 0.52 |
| (1,3319) | 1:61:A:VAL:HG11 | 1:65:A:ASN:HB3 | 2 | 0.52 |
| (1,3231) | 1:34:A:VAL:HG22 | 1:139:A:ASP:HA | 20 | 0.52 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 10 | 0.52 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 10 | 0.52 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 10 | 0.52 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 10 | 0.52 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 10 | 0.52 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 10 | 0.52 |
| (1,1075) | 1:48:A:VAL:H | 1:56:A:ALA:HB1 | 14 | 0.52 |
| (1,1075) | 1:48:A:VAL:H | 1:56:A:ALA:HB2 | 14 | 0.52 |
| (1,1075) | 1:48:A:VAL:H | 1:56:A:ALA:HB3 | 14 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 3 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 3 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 3 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 3 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 3 | 0.52 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 3 | 0.52 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 2 | 0.52 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 2 | 0.52 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 2 | 0.52 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 18 | 0.51 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 18 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 3 | 0.51 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 3 | 0.51 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 6 | 0.51 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 6 | 0.51 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB2 | 13 | 0.51 |
| (1,3582) | 1:17:A:LEU:HD11 | 1:191:A:PRO:HB3 | 13 | 0.51 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 19 | 0.51 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB2 | 10 | 0.51 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB3 | 10 | 0.51 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD2 | 13 | 0.51 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD3 | 13 | 0.51 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB1 | 14 | 0.51 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB2 | 14 | 0.51 |
| (1,3378) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB3 | 14 | 0.51 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 16 | 0.51 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 5 | 0.51 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 5 | 0.51 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 5 | 0.51 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 5 | 0.51 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 5 | 0.51 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 5 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD11 | 13 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD12 | 13 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD13 | 13 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD21 | 13 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD22 | 13 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD23 | 13 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD11 | 17 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD12 | 17 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD13 | 17 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD21 | 17 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD22 | 17 | 0.51 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD23 | 17 | 0.51 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD11 | 10 | 0.51 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD12 | 10 | 0.51 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD13 | 10 | 0.51 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD21 | 10 | 0.51 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD22 | 10 | 0.51 |
| (1,2226) | 1:59:A:LEU:HA | 1:59:A:LEU:HD23 | 10 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 9 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 9 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 9 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 9 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 9 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 9 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 15 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 15 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 15 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 15 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 15 | 0.51 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 15 | 0.51 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 5 | 0.51 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 5 | 0.51 |
| (1,3799) | 1:131:A:VAL:HG11 | 1:51:A:ALA:HA | 13 | 0.5 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 7 | 0.5 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 8 | 0.5 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 8 | 0.5 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 8 | 0.5 |
| (1,3553) | 1:87:A:ALA:HB2 | 1:43:A:ILE:HA | 1 | 0.5 |
| (1,3513) | 1:85:A:ALA:HB1 | 1:81:A:SER:HB2 | 7 | 0.5 |
| (1,3513) | 1:85:A:ALA:HB1 | 1:81:A:SER:HB3 | 7 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 3 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 3 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 3 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 3 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 3 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 3 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 19 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 19 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 19 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 19 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 19 | 0.5 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 19 | 0.5 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB2 | 5 | 0.5 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB3 | 5 | 0.5 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 1 | 0.5 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 12 | 0.5 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 1 | 0.5 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 1 | 0.5 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 6 | 0.5 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 6 | 0.5 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 6 | 0.5 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 9 | 0.5 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 9 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 9 | 0.5 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 9 | 0.5 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 9 | 0.5 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 9 | 0.5 |
| (1,3292) | 1:112:A:VAL:H | 1:108:A:LEU:HG | 9 | 0.5 |
| (1,3286) | 1:48:A:VAL:HG21 | 1:47:A:VAL:HB | 20 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 11 | 0.5 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 11 | 0.5 |
| (1,3268) | 1:9:A:ALA:HA | 1:113:A:LEU:HG | 9 | 0.5 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD11 | 4 | 0.5 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD12 | 4 | 0.5 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD13 | 4 | 0.5 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD21 | 4 | 0.5 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD22 | 4 | 0.5 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD23 | 4 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG11 | 2 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG12 | 2 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG13 | 2 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG21 | 2 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG22 | 2 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG23 | 2 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 9 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 9 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 9 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 9 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 9 | 0.5 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 9 | 0.5 |
| (1,1151) | 1:129:A:ILE:H | 1:130:A:ASN:H | 11 | 0.5 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 19 | 0.5 |
| (1,1063) | 1:126:A:GLY:H | 1:123:A:ALA:HB1 | 4 | 0.5 |
| (1,1063) | 1:126:A:GLY:H | 1:123:A:ALA:HB2 | 4 | 0.5 |
| (1,1063) | 1:126:A:GLY:H | 1:123:A:ALA:HB3 | 4 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB2 | 14 | 0.5 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB3 | 14 | 0.5 |
| (1,3791) | 1:44:A:ALA:HB3 | 1:74:A:VAL:HA | 11 | 0.49 |
| (1,3759) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB2 | 6 | 0.49 |
| (1,3759) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB3 | 6 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 13 | 0.49 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 13 | 0.49 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 18 | 0.49 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 18 | 0.49 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 18 | 0.49 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 19 | 0.49 |
| (1,3660) | 1:172:A:PRO:HG2 | 1:18:A:ILE:HG12 | 9 | 0.49 |
| (1,3660) | 1:172:A:PRO:HG2 | 1:18:A:ILE:HG13 | 9 | 0.49 |
| (1,3620) | 1:6:A:GLY:HA3 | 1:7:A:PHE:HA | 3 | 0.49 |
| (1,3589) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG12 | 20 | 0.49 |
| (1,3589) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG13 | 20 | 0.49 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 11 | 0.49 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 11 | 0.49 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 13 | 0.49 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 19 | 0.49 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 19 | 0.49 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 19 | 0.49 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 19 | 0.49 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 19 | 0.49 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 19 | 0.49 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 18 | 0.49 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 18 | 0.49 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD11 | 18 | 0.49 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD12 | 18 | 0.49 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD13 | 18 | 0.49 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD21 | 18 | 0.49 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD22 | 18 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD23 | 18 | 0.49 |
| (1,3292) | 1:112:A:VAL:H | 1:108:A:LEU:HG | 11 | 0.49 |
| (1,3231) | 1:34:A:VAL:HG21 | 1:139:A:ASP:HA | 8 | 0.49 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 16 | 0.49 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 16 | 0.49 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 15 | 0.49 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 18 | 0.49 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 18 | 0.49 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 18 | 0.49 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 18 | 0.49 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 18 | 0.49 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 18 | 0.49 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG11 | 5 | 0.49 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG12 | 5 | 0.49 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG13 | 5 | 0.49 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG21 | 5 | 0.49 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG22 | 5 | 0.49 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG23 | 5 | 0.49 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB2 | 4 | 0.49 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB3 | 4 | 0.49 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 10 | 0.48 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 10 | 0.48 |
| (1,3820) | 1:101:A:ASN:HB2 | 1:104:A:ASN:HB2 | 8 | 0.48 |
| (1,3820) | 1:101:A:ASN:HB2 | 1:104:A:ASN:HB3 | 8 | 0.48 |
| (1,3799) | 1:131:A:VAL:HG11 | 1:51:A:ALA:HA | 20 | 0.48 |
| (1,3796) | 1:124:A:ALA:HB3 | 1:120:A:VAL:HA | 4 | 0.48 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB1 | 13 | 0.48 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB2 | 13 | 0.48 |
| (1,3768) | 1:172:A:PRO:HG3 | 1:24:A:ALA:HB3 | 13 | 0.48 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG11 | 2 | 0.48 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG12 | 2 | 0.48 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG13 | 2 | 0.48 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG21 | 2 | 0.48 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG22 | 2 | 0.48 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG23 | 2 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 16 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 16 | 0.48 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 16 | 0.48 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG11 | 13 | 0.48 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG12 | 13 | 0.48 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG13 | 13 | 0.48 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG21 | 13 | 0.48 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG22 | 13 | 0.48 |
| (1,3679) | 1:70:A:ALA:HB1 | 1:61:A:VAL:HG23 | 13 | 0.48 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD11 | 3 | 0.48 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD12 | 3 | 0.48 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD13 | 3 | 0.48 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD21 | 3 | 0.48 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD22 | 3 | 0.48 |
| (1,3586) | 1:86:A:TYR:HB2 | 1:77:A:LEU:HD23 | 3 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD11 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD12 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG11 | 1:129:A:ILE:HD13 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD11 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD12 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG12 | 1:129:A:ILE:HD13 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD11 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD12 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG13 | 1:129:A:ILE:HD13 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD11 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD12 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG21 | 1:129:A:ILE:HD13 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD11 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD12 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG22 | 1:129:A:ILE:HD13 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD11 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD12 | 15 | 0.48 |
| (1,3416) | 1:39:A:VAL:HG23 | 1:129:A:ILE:HD13 | 15 | 0.48 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 19 | 0.48 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 20 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG11 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG12 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG13 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG21 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG22 | 19 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG23 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG11 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG12 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG13 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG21 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG22 | 19 | 0.48 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG23 | 19 | 0.48 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 2 | 0.48 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 2 | 0.48 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 2 | 0.48 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 17 | 0.48 |
| (1,3353) | 1:11:A:GLY:HA2 | 1:113:A:LEU:HA | 18 | 0.48 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB2 | 8 | 0.48 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB3 | 8 | 0.48 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB1 | 11 | 0.48 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB2 | 11 | 0.48 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB3 | 11 | 0.48 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG11 | 19 | 0.48 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG12 | 19 | 0.48 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG13 | 19 | 0.48 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG21 | 19 | 0.48 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG22 | 19 | 0.48 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG23 | 19 | 0.48 |
| (1,1065) | 1:111:A:ARG:HB2 | 1:111:A:ARG:HE | 17 | 0.48 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 18 | 0.48 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 18 | 0.48 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 18 | 0.48 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 13 | 0.48 |
| (1,3790) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 2 | 0.47 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB1 | 17 | 0.47 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB2 | 17 | 0.47 |
| (1,3785) | 1:158:A:GLN:HB2 | 1:161:A:ALA:HB3 | 17 | 0.47 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 20 | 0.47 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 20 | 0.47 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 20 | 0.47 |
| (1,3735) | 1:48:A:VAL:HG21 | 1:46:A:SER:H | 15 | 0.47 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 13 | 0.47 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 13 | 0.47 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 13 | 0.47 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 13 | 0.47 |
| (1,3657) | 1:77:A:LEU:HD13 | 1:73:A:ALA:HA | 4 | 0.47 |
| (1,3649) | 1:129:A:ILE:HG22 | 1:131:A:VAL:H | 18 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3647) | 1:35:A:LEU:HG | 1:131:A:VAL:HG11 | 10 | 0.47 |
| (1,3647) | 1:35:A:LEU:HG | 1:131:A:VAL:HG12 | 10 | 0.47 |
| (1,3647) | 1:35:A:LEU:HG | 1:131:A:VAL:HG13 | 10 | 0.47 |
| (1,3647) | 1:35:A:LEU:HG | 1:131:A:VAL:HG21 | 10 | 0.47 |
| (1,3647) | 1:35:A:LEU:HG | 1:131:A:VAL:HG22 | 10 | 0.47 |
| (1,3647) | 1:35:A:LEU:HG | 1:131:A:VAL:HG23 | 10 | 0.47 |
| (1,3620) | 1:6:A:GLY:HA3 | 1:7:A:PHE:HA | 5 | 0.47 |
| (1,3583) | 1:74:A:VAL:HG23 | 1:44:A:ALA:HA | 8 | 0.47 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 16 | 0.47 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 16 | 0.47 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 6 | 0.47 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 6 | 0.47 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 7 | 0.47 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 7 | 0.47 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 14 | 0.47 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 14 | 0.47 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 17 | 0.47 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 17 | 0.47 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 17 | 0.47 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 17 | 0.47 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 17 | 0.47 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 17 | 0.47 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 3 | 0.47 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 3 | 0.47 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 3 | 0.47 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 3 | 0.47 |
| (1,3286) | 1:48:A:VAL:HG22 | 1:47:A:VAL:HB | 7 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 5 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 10 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 10 | 0.47 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 10 | 0.47 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA2 | 16 | 0.47 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA3 | 16 | 0.47 |
| (1,1194) | 1:4:A:GLN:H | 1:7:A:PHE:HB2 | 6 | 0.47 |
| (1,1194) | 1:4:A:GLN:H | 1:7:A:PHE:HB3 | 6 | 0.47 |
| (1,1113) | 1:65:A:ASN:HD21 | 1:47:A:VAL:HB | 12 | 0.47 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 1 | 0.47 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 1 | 0.47 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 1 | 0.47 |
| (1,232) | 1:45:A:SER:HA | 1:47:A:VAL:H | 19 | 0.47 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 13 | 0.46 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 13 | 0.46 |
| (1,3712) | 1:84:A:SER:HB3 | 1:85:A:ALA:HA | 11 | 0.46 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD11 | 16 | 0.46 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD12 | 16 | 0.46 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD13 | 16 | 0.46 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD21 | 16 | 0.46 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD22 | 16 | 0.46 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD23 | 16 | 0.46 |
| (1,3620) | 1:6:A:GLY:HA3 | 1:7:A:PHE:HA | 18 | 0.46 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD11 | 1 | 0.46 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD12 | 1 | 0.46 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD13 | 1 | 0.46 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD21 | 1 | 0.46 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD22 | 1 | 0.46 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD23 | 1 | 0.46 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB2 | 17 | 0.46 |
| (1,3554) | 1:13:A:ALA:HB3 | 1:104:A:ASN:HB3 | 17 | 0.46 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 5 | 0.46 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 15 | 0.46 |
| (1,3422) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HB2 | 2 | 0.46 |
| (1,3422) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HB3 | 2 | 0.46 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB2 | 9 | 0.46 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB3 | 9 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 4 | 0.46 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 20 | 0.46 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 20 | 0.46 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 2 | 0.46 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB1 | 1 | 0.46 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB2 | 1 | 0.46 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB3 | 1 | 0.46 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB2 | 4 | 0.46 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB3 | 4 | 0.46 |
| (1,3231) | 1:34:A:VAL:HG22 | 1:139:A:ASP:HA | 10 | 0.46 |
| (1,2430) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HG | 16 | 0.46 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 18 | 0.46 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 18 | 0.46 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 12 | 0.46 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 12 | 0.46 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 14 | 0.46 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB1 | 19 | 0.46 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB2 | 19 | 0.46 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB3 | 19 | 0.46 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 15 | 0.46 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 15 | 0.46 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 14 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 14 | 0.45 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 14 | 0.45 |
| (1,3790) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 17 | 0.45 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB2 | 18 | 0.45 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB3 | 18 | 0.45 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB2 | 6 | 0.45 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB3 | 6 | 0.45 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA2 | 19 | 0.45 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA3 | 19 | 0.45 |
| (1,3645) | 1:25:A:LEU:HD11 | 1:180:A:SER:H | 19 | 0.45 |
| (1,3620) | 1:6:A:GLY:HA2 | 1:7:A:PHE:HA | 20 | 0.45 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 7 | 0.45 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 9 | 0.45 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG11 | 7 | 0.45 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG12 | 7 | 0.45 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG13 | 7 | 0.45 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG21 | 7 | 0.45 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG22 | 7 | 0.45 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:131:A:VAL:HG23 | 7 | 0.45 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD11 | 9 | 0.45 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD12 | 9 | 0.45 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD13 | 9 | 0.45 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD21 | 9 | 0.45 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD22 | 9 | 0.45 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD23 | 9 | 0.45 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 19 | 0.45 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 19 | 0.45 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 19 | 0.45 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 19 | 0.45 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 19 | 0.45 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 19 | 0.45 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 19 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 19 | 0.45 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 19 | 0.45 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 11 | 0.45 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 13 | 0.45 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 13 | 0.45 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 13 | 0.45 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 13 | 0.45 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 13 | 0.45 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 13 | 0.45 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 20 | 0.45 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 10 | 0.45 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 10 | 0.45 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 10 | 0.45 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 10 | 0.45 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 10 | 0.45 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 10 | 0.45 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD11 | 19 | 0.45 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD12 | 19 | 0.45 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD13 | 19 | 0.45 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD21 | 19 | 0.45 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD22 | 19 | 0.45 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD23 | 19 | 0.45 |
| (1,3106) | 1:154:A:ALA:HB1 | 1:158:A:GLN:HB2 | 5 | 0.45 |
| (1,3106) | 1:154:A:ALA:HB1 | 1:158:A:GLN:HB3 | 5 | 0.45 |
| (1,3106) | 1:154:A:ALA:HB2 | 1:158:A:GLN:HB2 | 5 | 0.45 |
| (1,3106) | 1:154:A:ALA:HB2 | 1:158:A:GLN:HB3 | 5 | 0.45 |
| (1,3106) | 1:154:A:ALA:HB3 | 1:158:A:GLN:HB2 | 5 | 0.45 |
| (1,3106) | 1:154:A:ALA:HB3 | 1:158:A:GLN:HB3 | 5 | 0.45 |
| (1,1662) | 1:132:A:ASP:HA | 1:133:A:SER:H | 19 | 0.45 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 11 | 0.45 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 11 | 0.45 |
| (1,1031) | 1:170:A:THR:HA | 1:169:A:TYR:H | 2 | 0.45 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 4 | 0.45 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 4 | 0.45 |
| (1,952) | 1:104:A:ASN:HD22 | 1:92:A:SER:HB2 | 8 | 0.45 |
| (1,952) | 1:104:A:ASN:HD22 | 1:92:A:SER:HB3 | 8 | 0.45 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB2 | 18 | 0.45 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB3 | 18 | 0.45 |
| (1,803) | 1:132:A:ASP:HA | 1:133:A:SER:H | 19 | 0.45 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 20 | 0.44 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 20 | 0.44 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 20 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 20 | 0.44 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 20 | 0.44 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 20 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 1 | 0.44 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 1 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 16 | 0.44 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 16 | 0.44 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB2 | 13 | 0.44 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB3 | 13 | 0.44 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB2 | 17 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB3 | 17 | 0.44 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 17 | 0.44 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 17 | 0.44 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 8 | 0.44 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 1 | 0.44 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 3 | 0.44 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 8 | 0.44 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 9 | 0.44 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 15 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB2 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB3 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB2 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB3 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB2 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB3 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB2 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB3 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB2 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB3 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB2 | 19 | 0.44 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB3 | 19 | 0.44 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 7 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 14 | 0.44 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 14 | 0.44 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 7 | 0.44 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 7 | 0.44 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB2 | 6 | 0.44 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB3 | 6 | 0.44 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 1 | 0.44 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 1 | 0.44 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 1 | 0.44 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 7 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 7 | 0.44 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 7 | 0.44 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 11 | 0.43 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 3 | 0.43 |
| (1,3712) | 1:84:A:SER:HB3 | 1:85:A:ALA:HA | 7 | 0.43 |
| (1,3695) | 1:195:A:SER:HB2 | 1:102:A:ALA:HA | 9 | 0.43 |
| (1,3654) | 1:39:A:VAL:HG11 | 1:38:A:GLY:HA2 | 19 | 0.43 |
| (1,3654) | 1:39:A:VAL:HG11 | 1:38:A:GLY:HA3 | 19 | 0.43 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 7 | 0.43 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 14 | 0.43 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG2 | 18 | 0.43 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG3 | 18 | 0.43 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 5 | 0.43 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 5 | 0.43 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 7 | 0.43 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 18 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG11 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG12 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG13 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG21 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG22 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG23 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG11 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG12 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG13 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG21 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG22 | 8 | 0.43 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG23 | 8 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG11 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG12 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG13 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG21 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG22 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB2 | 1:136:A:VAL:HG23 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG11 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG12 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG13 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG21 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG22 | 16 | 0.43 |
| (1,3376) | 1:132:A:ASP:HB3 | 1:136:A:VAL:HG23 | 16 | 0.43 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD11 | 20 | 0.43 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD12 | 20 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD13 | 20 | 0.43 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD21 | 20 | 0.43 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD22 | 20 | 0.43 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD23 | 20 | 0.43 |
| (1,3292) | 1:112:A:VAL:H | 1:108:A:LEU:HG | 1 | 0.43 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 9 | 0.43 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 9 | 0.43 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 9 | 0.43 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 20 | 0.43 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 20 | 0.43 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 20 | 0.43 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 17 | 0.43 |
| (1,989) | 1:110:A:SER:H | 1:117:A:LEU:HG | 5 | 0.43 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 14 | 0.43 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 11 | 0.43 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 11 | 0.43 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 11 | 0.43 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 11 | 0.43 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 11 | 0.43 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 11 | 0.43 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 15 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 6 | 0.42 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 6 | 0.42 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 19 | 0.42 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 19 | 0.42 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 19 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 19 | 0.42 |
| (1,3695) | 1:150:A:SER:HB3 | 1:147:A:LEU:HA | 7 | 0.42 |
| (1,3649) | 1:129:A:ILE:HG23 | 1:129:A:ILE:H | 12 | 0.42 |
| (1,3649) | 1:129:A:ILE:HG23 | 1:129:A:ILE:H | 19 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB2 | 1 | 0.42 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB3 | 1 | 0.42 |
| (1,3620) | 1:166:A:GLY:HA2 | 1:163:A:SER:HA | 6 | 0.42 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 16 | 0.42 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 16 | 0.42 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB1 | 13 | 0.42 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB2 | 13 | 0.42 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB3 | 13 | 0.42 |
| (1,3561) | 1:50:A:ARG:HD3 | 1:50:A:ARG:HA | 7 | 0.42 |
| (1,3553) | 1:87:A:ALA:HB1 | 1:43:A:ILE:HA | 5 | 0.42 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 10 | 0.42 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 10 | 0.42 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 10 | 0.42 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 10 | 0.42 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 10 | 0.42 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 10 | 0.42 |
| (1,3473) | 1:21:A:VAL:HG11 | 1:92:A:SER:HA | 20 | 0.42 |
| (1,3473) | 1:21:A:VAL:HG12 | 1:92:A:SER:HA | 20 | 0.42 |
| (1,3473) | 1:21:A:VAL:HG13 | 1:92:A:SER:HA | 20 | 0.42 |
| (1,3473) | 1:21:A:VAL:HG21 | 1:92:A:SER:HA | 20 | 0.42 |
| (1,3473) | 1:21:A:VAL:HG22 | 1:92:A:SER:HA | 20 | 0.42 |
| (1,3473) | 1:21:A:VAL:HG23 | 1:92:A:SER:HA | 20 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 2 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 2 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 2 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 3 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 3 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 3 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG21 | 5 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG22 | 5 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG23 | 5 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG21 | 6 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG22 | 6 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG23 | 6 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 11 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 11 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 11 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 12 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 12 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 12 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 13 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 13 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 13 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 14 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 14 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 14 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG21 | 15 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG22 | 15 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG23 | 15 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 16 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 16 | 0.42 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 16 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG21 | 19 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG22 | 19 | 0.42 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG23 | 19 | 0.42 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG2 | 11 | 0.42 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG3 | 11 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 12 | 0.42 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 12 | 0.42 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 8 | 0.42 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD2 | 10 | 0.42 |
| (1,3381) | 1:177:A:THR:HG21 | 1:179:A:PRO:HD3 | 10 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD11 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD12 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD13 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD21 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD22 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD23 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD11 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD12 | 4 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD13 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD21 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD22 | 4 | 0.42 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD23 | 4 | 0.42 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD11 | 7 | 0.42 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD12 | 7 | 0.42 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD13 | 7 | 0.42 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD21 | 7 | 0.42 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD22 | 7 | 0.42 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD23 | 7 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE1 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE2 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE1 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE2 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE1 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE2 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE1 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE2 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE1 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE2 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE1 | 8 | 0.42 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE2 | 8 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG11 | 1:49:A:GLN:HG2 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG11 | 1:49:A:GLN:HG3 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG12 | 1:49:A:GLN:HG2 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG12 | 1:49:A:GLN:HG3 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG13 | 1:49:A:GLN:HG2 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG13 | 1:49:A:GLN:HG3 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG21 | 1:49:A:GLN:HG2 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG21 | 1:49:A:GLN:HG3 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG22 | 1:49:A:GLN:HG2 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG22 | 1:49:A:GLN:HG3 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG23 | 1:49:A:GLN:HG2 | 9 | 0.42 |
| (1,2144) | 1:47:A:VAL:HG23 | 1:49:A:GLN:HG3 | 9 | 0.42 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 10 | 0.42 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 18 | 0.42 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 14 | 0.42 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 14 | 0.42 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 14 | 0.42 |
| (1,1039) | 1:90:A:PHE:H | 1:18:A:ILE:HB | 1 | 0.42 |
| (1,989) | 1:110:A:SER:H | 1:117:A:LEU:HG | 2 | 0.42 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD11 | 8 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD12 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD13 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD21 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD22 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD23 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD11 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD12 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD13 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD21 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD22 | 8 | 0.42 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD23 | 8 | 0.42 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 12 | 0.41 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 12 | 0.41 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 12 | 0.41 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 12 | 0.41 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 12 | 0.41 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 12 | 0.41 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 16 | 0.41 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 16 | 0.41 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 16 | 0.41 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 16 | 0.41 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 16 | 0.41 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 16 | 0.41 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 5 | 0.41 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 5 | 0.41 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 5 | 0.41 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD11 | 19 | 0.41 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD12 | 19 | 0.41 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD13 | 19 | 0.41 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD21 | 19 | 0.41 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD22 | 19 | 0.41 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD23 | 19 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 2 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 2 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 2 | 0.41 |
| (1,3712) | 1:84:A:SER:HB3 | 1:85:A:ALA:HA | 17 | 0.41 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 7 | 0.41 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 7 | 0.41 |
| (1,3649) | 1:129:A:ILE:HG21 | 1:129:A:ILE:H | 15 | 0.41 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB2 | 8 | 0.41 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB3 | 8 | 0.41 |
| (1,3620) | 1:6:A:GLY:HA3 | 1:7:A:PHE:HA | 9 | 0.41 |
| (1,3620) | 1:6:A:GLY:HA3 | 1:7:A:PHE:HA | 16 | 0.41 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 17 | 0.41 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 17 | 0.41 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 17 | 0.41 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 17 | 0.41 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 17 | 0.41 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 17 | 0.41 |
| (1,3473) | 1:21:A:VAL:HG11 | 1:92:A:SER:HA | 10 | 0.41 |
| (1,3473) | 1:21:A:VAL:HG12 | 1:92:A:SER:HA | 10 | 0.41 |
| (1,3473) | 1:21:A:VAL:HG13 | 1:92:A:SER:HA | 10 | 0.41 |
| (1,3473) | 1:21:A:VAL:HG21 | 1:92:A:SER:HA | 10 | 0.41 |
| (1,3473) | 1:21:A:VAL:HG22 | 1:92:A:SER:HA | 10 | 0.41 |
| (1,3473) | 1:21:A:VAL:HG23 | 1:92:A:SER:HA | 10 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 1 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 1 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 1 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 4 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 4 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 4 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 7 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 7 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 7 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 9 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 9 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 9 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 10 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 10 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 10 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 18 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 18 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 18 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 20 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 20 | 0.41 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 20 | 0.41 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 13 | 0.41 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 13 | 0.41 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB2 | 12 | 0.41 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HB3 | 12 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG2 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG3 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG2 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG3 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG2 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG3 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG2 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG3 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG2 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG3 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG2 | 4 | 0.41 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG3 | 4 | 0.41 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 4 | 0.41 |
| (1,3415) | 1:97:A:ALA:HA | 1:96:A:ASN:HA | 10 | 0.41 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 9 | 0.41 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 9 | 0.41 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 9 | 0.41 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 9 | 0.41 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 9 | 0.41 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 9 | 0.41 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 8 | 0.41 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 8 | 0.41 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HB2 | 1 | 0.41 |
| (1,3295) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HB3 | 1 | 0.41 |
| (1,3268) | 1:9:A:ALA:HA | 1:113:A:LEU:HG | 15 | 0.41 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA2 | 6 | 0.41 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA3 | 6 | 0.41 |
| (1,3231) | 1:34:A:VAL:HG22 | 1:139:A:ASP:HA | 15 | 0.41 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD11 | 17 | 0.41 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD12 | 17 | 0.41 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD13 | 17 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD21 | 17 | 0.41 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD22 | 17 | 0.41 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD23 | 17 | 0.41 |
| (1,3194) | 1:190:A:ALA:HB1 | 1:192:A:PHE:HA | 19 | 0.41 |
| (1,3194) | 1:190:A:ALA:HB2 | 1:192:A:PHE:HA | 19 | 0.41 |
| (1,3194) | 1:190:A:ALA:HB3 | 1:192:A:PHE:HA | 19 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 14 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 14 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 14 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 14 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 14 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 14 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 15 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 15 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 15 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 15 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 15 | 0.41 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 15 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 6 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 6 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 6 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 6 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 6 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 6 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 12 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 12 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 12 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 12 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 12 | 0.41 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 12 | 0.41 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 16 | 0.41 |
| (1,1123) | 1:132:A:ASP:H | 1:136:A:VAL:HB | 9 | 0.41 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB1 | 15 | 0.41 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB2 | 15 | 0.41 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB3 | 15 | 0.41 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 6 | 0.41 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 6 | 0.41 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 6 | 0.41 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 6 | 0.41 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 6 | 0.41 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 6 | 0.41 |
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 9 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 15 | 0.41 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 6 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 11 | 0.4 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 11 | 0.4 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 17 | 0.4 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 17 | 0.4 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 17 | 0.4 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 7 | 0.4 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 8 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB2 | 8 | 0.4 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB3 | 8 | 0.4 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD11 | 16 | 0.4 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD12 | 16 | 0.4 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD13 | 16 | 0.4 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD21 | 16 | 0.4 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD22 | 16 | 0.4 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD23 | 16 | 0.4 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB2 | 11 | 0.4 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB3 | 11 | 0.4 |
| (1,3620) | 1:193:A:GLY:HA2 | 1:192:A:PHE:HA | 14 | 0.4 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE21 | 2 | 0.4 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE22 | 2 | 0.4 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 18 | 0.4 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 18 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB1 | 10 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB2 | 10 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB3 | 10 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB1 | 10 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB2 | 10 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB3 | 10 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB1 | 11 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB2 | 11 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE21 | 1:44:A:ALA:HB3 | 11 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB1 | 11 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB2 | 11 | 0.4 |
| (1,3574) | 1:41:A:GLN:HE22 | 1:44:A:ALA:HB3 | 11 | 0.4 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB2 | 13 | 0.4 |
| (1,3554) | 1:13:A:ALA:HB1 | 1:104:A:ASN:HB3 | 13 | 0.4 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG21 | 8 | 0.4 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG22 | 8 | 0.4 |
| (1,3469) | 1:33:A:THR:HA | 1:33:A:THR:HG23 | 8 | 0.4 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 2 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 5 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 5 | 0.4 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 5 | 0.4 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 16 | 0.4 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 16 | 0.4 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 16 | 0.4 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 16 | 0.4 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 16 | 0.4 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 16 | 0.4 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD11 | 11 | 0.4 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD12 | 11 | 0.4 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD13 | 11 | 0.4 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD21 | 11 | 0.4 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD22 | 11 | 0.4 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD23 | 11 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 17 | 0.4 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 17 | 0.4 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA2 | 1 | 0.4 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA3 | 1 | 0.4 |
| (1,3231) | 1:34:A:VAL:HG22 | 1:139:A:ASP:HA | 17 | 0.4 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 17 | 0.4 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 17 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 5 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 5 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 5 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 5 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 5 | 0.4 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 5 | 0.4 |
| (1,1113) | 1:65:A:ASN:HD21 | 1:47:A:VAL:HB | 17 | 0.4 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB1 | 2 | 0.4 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB2 | 2 | 0.4 |
| (1,1070) | 1:67:A:ALA:H | 1:70:A:ALA:HB3 | 2 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 19 | 0.4 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 19 | 0.4 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 19 | 0.4 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 1 | 0.4 |
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 1 | 0.4 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 19 | 0.4 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 9 | 0.4 |
| (1,989) | 1:110:A:SER:H | 1:117:A:LEU:HG | 18 | 0.4 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 11 | 0.39 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 11 | 0.39 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 11 | 0.39 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 11 | 0.39 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 11 | 0.39 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 11 | 0.39 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 11 | 0.39 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 11 | 0.39 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 1 | 0.39 |
| (1,3799) | 1:131:A:VAL:HG12 | 1:51:A:ALA:HA | 2 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 13 | 0.39 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 13 | 0.39 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 10 | 0.39 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 10 | 0.39 |
| (1,3649) | 1:129:A:ILE:HG23 | 1:129:A:ILE:H | 11 | 0.39 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 11 | 0.39 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 11 | 0.39 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 12 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 12 | 0.39 |
| (1,3543) | 1:17:A:LEU:HD13 | 1:93:A:ALA:HA | 8 | 0.39 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD11 | 2 | 0.39 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD12 | 2 | 0.39 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD13 | 2 | 0.39 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD21 | 2 | 0.39 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD22 | 2 | 0.39 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD23 | 2 | 0.39 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 16 | 0.39 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 16 | 0.39 |
| (1,3319) | 1:61:A:VAL:HG23 | 1:65:A:ASN:HB2 | 17 | 0.39 |
| (1,3319) | 1:61:A:VAL:HG23 | 1:65:A:ASN:HB3 | 17 | 0.39 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 6 | 0.39 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 6 | 0.39 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB1 | 3 | 0.39 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB2 | 3 | 0.39 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB3 | 3 | 0.39 |
| (1,2430) | 1:43:A:ILE:HD12 | 1:77:A:LEU:HG | 11 | 0.39 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 20 | 0.39 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 14 | 0.39 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 8 | 0.39 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 1 | 0.39 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 13 | 0.38 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 13 | 0.38 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 13 | 0.38 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 13 | 0.38 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 13 | 0.38 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 13 | 0.38 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 6 | 0.38 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 6 | 0.38 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 6 | 0.38 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB2 | 2 | 0.38 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB3 | 2 | 0.38 |
| (1,3799) | 1:131:A:VAL:HG11 | 1:51:A:ALA:HA | 3 | 0.38 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 15 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 5 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 5 | 0.38 |
| (1,3754) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 5 | 0.38 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 1 | 0.38 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 1 | 0.38 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 16 | 0.38 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 16 | 0.38 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 17 | 0.38 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 17 | 0.38 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 16 | 0.38 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 16 | 0.38 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB1 | 12 | 0.38 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB2 | 12 | 0.38 |
| (1,3580) | 1:104:A:ASN:HB3 | 1:102:A:ALA:HB3 | 12 | 0.38 |
| (1,3561) | 1:50:A:ARG:HD2 | 1:50:A:ARG:HA | 11 | 0.38 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG21 | 17 | 0.38 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG22 | 17 | 0.38 |
| (1,3469) | 1:58:A:THR:HA | 1:58:A:THR:HG23 | 17 | 0.38 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG2 | 20 | 0.38 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG3 | 20 | 0.38 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 12 | 0.38 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 15 | 0.38 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD11 | 7 | 0.38 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD12 | 7 | 0.38 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD13 | 7 | 0.38 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD21 | 7 | 0.38 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD22 | 7 | 0.38 |
| (1,3348) | 1:140:A:ILE:H | 1:35:A:LEU:HD23 | 7 | 0.38 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD11 | 3 | 0.38 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD12 | 3 | 0.38 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD13 | 3 | 0.38 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD21 | 3 | 0.38 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD22 | 3 | 0.38 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD23 | 3 | 0.38 |
| (1,3238) | 1:129:A:ILE:HD13 | 1:128:A:GLY:HA2 | 13 | 0.38 |
| (1,3238) | 1:129:A:ILE:HD13 | 1:128:A:GLY:HA3 | 13 | 0.38 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG21 | 2 | 0.38 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG22 | 2 | 0.38 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG23 | 2 | 0.38 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG21 | 2 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG22 | 2 | 0.38 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG23 | 2 | 0.38 |
| (1,1904) | 1:20:A:ARG:HA | 1:24:A:ALA:HA | 3 | 0.38 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 19 | 0.38 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 19 | 0.38 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 20 | 0.38 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 20 | 0.38 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 20 | 0.38 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 20 | 0.38 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 20 | 0.38 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 20 | 0.38 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 9 | 0.38 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 18 | 0.38 |
| (1,1138) | 1:147:A:LEU:HB3 | 1:149:A:THR:H | 12 | 0.38 |
| (1,1095) | 1:193:A:GLY:H | 1:191:A:PRO:HA | 12 | 0.38 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD11 | 16 | 0.38 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD12 | 16 | 0.38 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD13 | 16 | 0.38 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD21 | 16 | 0.38 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD22 | 16 | 0.38 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD23 | 16 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 7 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 7 | 0.38 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 7 | 0.38 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 14 | 0.38 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 14 | 0.38 |
| (1,919) | 1:180:A:SER:H | 1:180:A:SER:HB2 | 6 | 0.38 |
| (1,919) | 1:180:A:SER:H | 1:180:A:SER:HB3 | 6 | 0.38 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 4 | 0.37 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 4 | 0.37 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD11 | 8 | 0.37 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD12 | 8 | 0.37 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD13 | 8 | 0.37 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD21 | 8 | 0.37 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD22 | 8 | 0.37 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD23 | 8 | 0.37 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 10 | 0.37 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 6 | 0.37 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 6 | 0.37 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 14 | 0.37 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 14 | 0.37 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB2 | 10 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB3 | 10 | 0.37 |
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB2 | 15 | 0.37 |
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB3 | 15 | 0.37 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA2 | 18 | 0.37 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA3 | 18 | 0.37 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD11 | 17 | 0.37 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD12 | 17 | 0.37 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD13 | 17 | 0.37 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD21 | 17 | 0.37 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD22 | 17 | 0.37 |
| (1,3579) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HD23 | 17 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 2 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 2 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 2 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 2 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 2 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 2 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 8 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 8 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 8 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 8 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 8 | 0.37 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 8 | 0.37 |
| (1,3559) | 1:156:A:TYR:HA | 1:155:A:SER:HB2 | 16 | 0.37 |
| (1,3559) | 1:156:A:TYR:HA | 1:155:A:SER:HB3 | 16 | 0.37 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 16 | 0.37 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 16 | 0.37 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 16 | 0.37 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 16 | 0.37 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 16 | 0.37 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 16 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG11 | 1:92:A:SER:HA | 12 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG12 | 1:92:A:SER:HA | 12 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG13 | 1:92:A:SER:HA | 12 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG21 | 1:92:A:SER:HA | 12 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG22 | 1:92:A:SER:HA | 12 | 0.37 |
| (1,3473) | 1:21:A:VAL:HG23 | 1:92:A:SER:HA | 12 | 0.37 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB2 | 14 | 0.37 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:66:A:LEU:HB3 | 14 | 0.37 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB2 | 17 | 0.37 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB3 | 17 | 0.37 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 14 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 4 | 0.37 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 4 | 0.37 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 4 | 0.37 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 2 | 0.37 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 10 | 0.37 |
| (1,1095) | 1:193:A:GLY:H | 1:194:A:GLN:HA | 8 | 0.37 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD11 | 12 | 0.37 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD12 | 12 | 0.37 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD13 | 12 | 0.37 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD21 | 12 | 0.37 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD22 | 12 | 0.37 |
| (1,1077) | 1:92:A:SER:H | 1:100:A:LEU:HD23 | 12 | 0.37 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 8 | 0.37 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 18 | 0.37 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG21 | 15 | 0.37 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG22 | 15 | 0.37 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG23 | 15 | 0.37 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 9 | 0.37 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 9 | 0.37 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 9 | 0.37 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 18 | 0.37 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 5 | 0.37 |
| (1,999) | 1:134:A:GLY:HA2 | 1:132:A:ASP:H | 3 | 0.37 |
| (1,999) | 1:134:A:GLY:HA3 | 1:132:A:ASP:H | 3 | 0.37 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 6 | 0.37 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 2 | 0.37 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 12 | 0.37 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 12 | 0.37 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 3 | 0.36 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 3 | 0.36 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 3 | 0.36 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 3 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 3 | 0.36 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 3 | 0.36 |
| (1,3840) | 1:125:A:GLN:HA | 1:97:A:ALA:HA | 3 | 0.36 |
| (1,3820) | 1:101:A:ASN:HB2 | 1:104:A:ASN:HB2 | 15 | 0.36 |
| (1,3820) | 1:101:A:ASN:HB2 | 1:104:A:ASN:HB3 | 15 | 0.36 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 2 | 0.36 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB2 | 7 | 0.36 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB3 | 7 | 0.36 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG21 | 14 | 0.36 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG22 | 14 | 0.36 |
| (1,3753) | 1:15:A:ALA:HB3 | 1:18:A:ILE:HG23 | 14 | 0.36 |
| (1,3748) | 1:36:A:ARG:HD2 | 1:91:A:SER:HB2 | 3 | 0.36 |
| (1,3748) | 1:36:A:ARG:HD2 | 1:91:A:SER:HB3 | 3 | 0.36 |
| (1,3712) | 1:84:A:SER:HB3 | 1:85:A:ALA:HA | 13 | 0.36 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB2 | 13 | 0.36 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB3 | 13 | 0.36 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD11 | 2 | 0.36 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD12 | 2 | 0.36 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD13 | 2 | 0.36 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD21 | 2 | 0.36 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD22 | 2 | 0.36 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD23 | 2 | 0.36 |
| (1,3649) | 1:129:A:ILE:HG23 | 1:131:A:VAL:H | 5 | 0.36 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD11 | 3 | 0.36 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD12 | 3 | 0.36 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD13 | 3 | 0.36 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD21 | 3 | 0.36 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD22 | 3 | 0.36 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD23 | 3 | 0.36 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 15 | 0.36 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 15 | 0.36 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 1 | 0.36 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 1 | 0.36 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 1 | 0.36 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 1 | 0.36 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 1 | 0.36 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 1 | 0.36 |
| (1,3561) | 1:50:A:ARG:HD2 | 1:50:A:ARG:HA | 6 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 2 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 2 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 2 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 2 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 2 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 2 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 5 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 5 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 5 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 5 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 5 | 0.36 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 5 | 0.36 |
| (1,3474) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HB2 | 5 | 0.36 |
| (1,3474) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HB3 | 5 | 0.36 |
| (1,3474) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HB2 | 5 | 0.36 |
| (1,3474) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HB3 | 5 | 0.36 |
| (1,3474) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HB2 | 5 | 0.36 |
| (1,3474) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HB3 | 5 | 0.36 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB2 | 15 | 0.36 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB3 | 15 | 0.36 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD11 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD12 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG21 | 1:129:A:ILE:HD13 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD11 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD12 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG22 | 1:129:A:ILE:HD13 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD11 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD12 | 14 | 0.36 |
| (1,3416) | 1:37:A:THR:HG23 | 1:129:A:ILE:HD13 | 14 | 0.36 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD11 | 20 | 0.36 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD12 | 20 | 0.36 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD13 | 20 | 0.36 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD21 | 20 | 0.36 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD22 | 20 | 0.36 |
| (1,3348) | 1:132:A:ASP:H | 1:35:A:LEU:HD23 | 20 | 0.36 |
| (1,3334) | 1:25:A:LEU:HA | 1:190:A:ALA:HA | 10 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD11 | 11 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD12 | 11 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD13 | 11 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD21 | 11 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD22 | 11 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:66:A:LEU:HD23 | 11 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB1 | 1:129:A:ILE:HD11 | 14 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB1 | 1:129:A:ILE:HD12 | 14 | 0.36 |
| (1,3332) | 1:52:A:ALA:HB1 | 1:129:A:ILE:HD13 | 14 | 0.36 |
| (1,3095) | 1:146:A:PHE:HB2 | 1:150:A:SER:HA | 11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3095) | 1:146:A:PHE:HB3 | 1:150:A:SER:HA | 11 | 0.36 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 8 | 0.36 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 8 | 0.36 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 7 | 0.36 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 14 | 0.36 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 14 | 0.36 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 14 | 0.36 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 14 | 0.36 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 14 | 0.36 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 14 | 0.36 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 20 | 0.36 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 20 | 0.36 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 20 | 0.36 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 11 | 0.36 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 3 | 0.36 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 9 | 0.36 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 11 | 0.36 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 11 | 0.36 |
| (1,989) | 1:110:A:SER:H | 1:117:A:LEU:HG | 4 | 0.36 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 16 | 0.36 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 1 | 0.35 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 1 | 0.35 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 1 | 0.35 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 1 | 0.35 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 1 | 0.35 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 1 | 0.35 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 7 | 0.35 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 7 | 0.35 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 7 | 0.35 |
| (1,3798) | 1:161:A:ALA:HA | 1:153:A:SER:HA | 13 | 0.35 |
| (1,3793) | 1:48:A:VAL:HG23 | 1:65:A:ASN:HD21 | 1 | 0.35 |
| (1,3793) | 1:48:A:VAL:HG23 | 1:65:A:ASN:HD22 | 1 | 0.35 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD21 | 13 | 0.35 |
| (1,3793) | 1:48:A:VAL:HG21 | 1:65:A:ASN:HD22 | 13 | 0.35 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG2 | 17 | 0.35 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG3 | 17 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD11 | 1:120:A:VAL:HG11 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD11 | 1:120:A:VAL:HG12 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD11 | 1:120:A:VAL:HG13 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD11 | 1:120:A:VAL:HG21 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD11 | 1:120:A:VAL:HG22 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD11 | 1:120:A:VAL:HG23 | 14 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3766) | 1:105:A:ILE:HD12 | 1:120:A:VAL:HG11 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD12 | 1:120:A:VAL:HG12 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD12 | 1:120:A:VAL:HG13 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD12 | 1:120:A:VAL:HG21 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD12 | 1:120:A:VAL:HG22 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD12 | 1:120:A:VAL:HG23 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD13 | 1:120:A:VAL:HG11 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD13 | 1:120:A:VAL:HG12 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD13 | 1:120:A:VAL:HG13 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD13 | 1:120:A:VAL:HG21 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD13 | 1:120:A:VAL:HG22 | 14 | 0.35 |
| (1,3766) | 1:105:A:ILE:HD13 | 1:120:A:VAL:HG23 | 14 | 0.35 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 12 | 0.35 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 12 | 0.35 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 1 | 0.35 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 1 | 0.35 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 2 | 0.35 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 2 | 0.35 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 2 | 0.35 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 2 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:14:A:SER:HB2 | 1 | 0.35 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:14:A:SER:HB3 | 1 | 0.35 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 20 | 0.35 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 20 | 0.35 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 20 | 0.35 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 20 | 0.35 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 20 | 0.35 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 20 | 0.35 |
| (1,3464) | 1:134:A:GLY:HA2 | 1:133:A:SER:HA | 6 | 0.35 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB2 | 1 | 0.35 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB3 | 1 | 0.35 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD2 | 6 | 0.35 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD3 | 6 | 0.35 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB2 | 15 | 0.35 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB3 | 15 | 0.35 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB2 | 7 | 0.35 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB3 | 7 | 0.35 |
| (1,3286) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HB2 | 1 | 0.35 |
| (1,3286) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HB3 | 1 | 0.35 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA2 | 18 | 0.35 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA3 | 18 | 0.35 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG2 | 8 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG3 | 8 | 0.35 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG2 | 8 | 0.35 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG3 | 8 | 0.35 |
| (1,3106) | 1:154:A:ALA:HB1 | 1:158:A:GLN:HB2 | 4 | 0.35 |
| (1,3106) | 1:154:A:ALA:HB1 | 1:158:A:GLN:HB3 | 4 | 0.35 |
| (1,3106) | 1:154:A:ALA:HB2 | 1:158:A:GLN:HB2 | 4 | 0.35 |
| (1,3106) | 1:154:A:ALA:HB2 | 1:158:A:GLN:HB3 | 4 | 0.35 |
| (1,3106) | 1:154:A:ALA:HB3 | 1:158:A:GLN:HB2 | 4 | 0.35 |
| (1,3106) | 1:154:A:ALA:HB3 | 1:158:A:GLN:HB3 | 4 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 11 | 0.35 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 11 | 0.35 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 12 | 0.35 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG11 | 2 | 0.35 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG12 | 2 | 0.35 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG13 | 2 | 0.35 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG21 | 2 | 0.35 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG22 | 2 | 0.35 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG23 | 2 | 0.35 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 11 | 0.35 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 13 | 0.35 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 17 | 0.35 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 14 | 0.35 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 14 | 0.35 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 14 | 0.35 |
| (1,1065) | 1:50:A:ARG:HB2 | 1:50:A:ARG:HE | 5 | 0.35 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG11 | 3 | 0.35 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG12 | 3 | 0.35 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG13 | 3 | 0.35 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG21 | 3 | 0.35 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG22 | 3 | 0.35 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG23 | 3 | 0.35 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 8 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 9 | 0.35 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 9 | 0.35 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 9 | 0.35 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 9 | 0.35 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 9 | 0.35 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 9 | 0.35 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD11 | 3 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD12 | 3 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD13 | 3 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD21 | 3 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD22 | 3 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD23 | 3 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD11 | 18 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD12 | 18 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD13 | 18 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD21 | 18 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD22 | 18 | 0.34 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD23 | 18 | 0.34 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG2 | 7 | 0.34 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG3 | 7 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG11 | 5 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG12 | 5 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG13 | 5 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG21 | 5 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG22 | 5 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD2 | 1:112:A:VAL:HG23 | 5 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 17 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 17 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 17 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 17 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 17 | 0.34 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 17 | 0.34 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB2 | 8 | 0.34 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB3 | 8 | 0.34 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 9 | 0.34 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 9 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 7 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 7 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 7 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 7 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 8 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 8 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 8 | 0.34 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 8 | 0.34 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA2 | 13 | 0.34 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA3 | 13 | 0.34 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:12:A:GLY:HA2 | 15 | 0.34 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:12:A:GLY:HA3 | 15 | 0.34 |
| (1,3583) | 1:74:A:VAL:HG23 | 1:44:A:ALA:HA | 7 | 0.34 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 3 | 0.34 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 3 | 0.34 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 3 | 0.34 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 3 | 0.34 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 3 | 0.34 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 3 | 0.34 |
| (1,3459) | 1:35:A:LEU:HD23 | 1:136:A:VAL:HG11 | 3 | 0.34 |
| (1,3459) | 1:35:A:LEU:HD23 | 1:136:A:VAL:HG12 | 3 | 0.34 |
| (1,3459) | 1:35:A:LEU:HD23 | 1:136:A:VAL:HG13 | 3 | 0.34 |
| (1,3459) | 1:35:A:LEU:HD23 | 1:136:A:VAL:HG21 | 3 | 0.34 |
| (1,3459) | 1:35:A:LEU:HD23 | 1:136:A:VAL:HG22 | 3 | 0.34 |
| (1,3459) | 1:35:A:LEU:HD23 | 1:136:A:VAL:HG23 | 3 | 0.34 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB2 | 6 | 0.34 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB3 | 6 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 11 | 0.34 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 11 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB1 | 1 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB2 | 1 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB3 | 1 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB1 | 7 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB2 | 7 | 0.34 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB3 | 7 | 0.34 |
| (1,3374) | 1:93:A:ALA:HB2 | 1:90:A:PHE:HA | 18 | 0.34 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 9 | 0.34 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 9 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 9 | 0.34 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB2 | 12 | 0.34 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB3 | 12 | 0.34 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 14 | 0.34 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 14 | 0.34 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA2 | 12 | 0.34 |
| (1,3238) | 1:129:A:ILE:HD12 | 1:128:A:GLY:HA3 | 12 | 0.34 |
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 15 | 0.34 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 6 | 0.34 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 6 | 0.34 |
| (1,1107) | 1:109:A:GLY:H | 1:112:A:VAL:HB | 1 | 0.34 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 1 | 0.34 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 4 | 0.34 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 7 | 0.34 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 13 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG11 | 13 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG12 | 13 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG13 | 13 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG21 | 13 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG22 | 13 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG23 | 13 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 15 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 15 | 0.34 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 15 | 0.34 |
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 19 | 0.34 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 19 | 0.34 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 19 | 0.34 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 19 | 0.34 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 19 | 0.34 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 19 | 0.34 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 19 | 0.34 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG11 | 3 | 0.34 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG12 | 3 | 0.34 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG13 | 3 | 0.34 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG21 | 3 | 0.34 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG22 | 3 | 0.34 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG23 | 3 | 0.34 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 3 | 0.34 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 17 | 0.34 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 12 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 12 | 0.33 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 12 | 0.33 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 17 | 0.33 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG2 | 20 | 0.33 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG3 | 20 | 0.33 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB2 | 10 | 0.33 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB3 | 10 | 0.33 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 6 | 0.33 |
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB2 | 6 | 0.33 |
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB3 | 6 | 0.33 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB2 | 5 | 0.33 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB3 | 5 | 0.33 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB2 | 19 | 0.33 |
| (1,3696) | 1:129:A:ILE:HG21 | 1:50:A:ARG:HB3 | 19 | 0.33 |
| (1,3683) | 1:56:A:ALA:HB2 | 1:50:A:ARG:HA | 6 | 0.33 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:12:A:GLY:HA2 | 6 | 0.33 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:12:A:GLY:HA3 | 6 | 0.33 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 8 | 0.33 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 8 | 0.33 |
| (1,3620) | 1:6:A:GLY:HA3 | 1:7:A:PHE:HA | 19 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB1 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB2 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB3 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB1 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB2 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB3 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB1 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB2 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB3 | 10 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB1 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB2 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB3 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB1 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB2 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB3 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB1 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB2 | 10 | 0.33 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB3 | 10 | 0.33 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB1 | 2 | 0.33 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB2 | 2 | 0.33 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB3 | 2 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 1 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 1 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 1 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 1 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 1 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 1 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 12 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 12 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 12 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 12 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 12 | 0.33 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 12 | 0.33 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 11 | 0.33 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 11 | 0.33 |
| (1,3473) | 1:21:A:VAL:HG11 | 1:92:A:SER:HA | 5 | 0.33 |
| (1,3473) | 1:21:A:VAL:HG12 | 1:92:A:SER:HA | 5 | 0.33 |
| (1,3473) | 1:21:A:VAL:HG13 | 1:92:A:SER:HA | 5 | 0.33 |
| (1,3473) | 1:21:A:VAL:HG21 | 1:92:A:SER:HA | 5 | 0.33 |
| (1,3473) | 1:21:A:VAL:HG22 | 1:92:A:SER:HA | 5 | 0.33 |
| (1,3473) | 1:21:A:VAL:HG23 | 1:92:A:SER:HA | 5 | 0.33 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD2 | 8 | 0.33 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD3 | 8 | 0.33 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD11 | 14 | 0.33 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD12 | 14 | 0.33 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD13 | 14 | 0.33 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD21 | 14 | 0.33 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD22 | 14 | 0.33 |
| (1,3320) | 1:99:A:VAL:HG21 | 1:100:A:LEU:HD23 | 14 | 0.33 |
| (1,3225) | 1:120:A:VAL:HB | 1:116:A:LEU:HG | 13 | 0.33 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD11 | 6 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD12 | 6 | 0.33 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD13 | 6 | 0.33 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD21 | 6 | 0.33 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD22 | 6 | 0.33 |
| (1,3220) | 1:9:A:ALA:HB3 | 1:117:A:LEU:HD23 | 6 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 12 | 0.33 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 12 | 0.33 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 3 | 0.33 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 5 | 0.33 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 5 | 0.33 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 16 | 0.33 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG21 | 19 | 0.33 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG22 | 19 | 0.33 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG23 | 19 | 0.33 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 5 | 0.33 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 5 | 0.33 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 5 | 0.33 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 10 | 0.33 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 10 | 0.33 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 10 | 0.33 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 16 | 0.33 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 16 | 0.33 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 16 | 0.33 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 16 | 0.33 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 16 | 0.33 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 16 | 0.33 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 19 | 0.33 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 12 | 0.33 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 12 | 0.33 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 13 | 0.33 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 13 | 0.33 |
| (1,961) | 1:10:A:THR:H | 1:113:A:LEU:H | 5 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB2 | 11 | 0.33 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB3 | 11 | 0.33 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 16 | 0.32 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 16 | 0.32 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 16 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD11 | 16 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD12 | 16 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD13 | 16 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD21 | 16 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD22 | 16 | 0.32 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD23 | 16 | 0.32 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 4 | 0.32 |
| (1,3798) | 1:164:A:THR:HB | 1:162:A:SER:HA | 9 | 0.32 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 12 | 0.32 |
| (1,3793) | 1:48:A:VAL:HG22 | 1:65:A:ASN:HD21 | 16 | 0.32 |
| (1,3793) | 1:48:A:VAL:HG22 | 1:65:A:ASN:HD22 | 16 | 0.32 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG2 | 3 | 0.32 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG3 | 3 | 0.32 |
| (1,3707) | 1:86:A:TYR:HB2 | 1:43:A:ILE:HG21 | 10 | 0.32 |
| (1,3707) | 1:86:A:TYR:HB2 | 1:43:A:ILE:HG22 | 10 | 0.32 |
| (1,3707) | 1:86:A:TYR:HB2 | 1:43:A:ILE:HG23 | 10 | 0.32 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA2 | 16 | 0.32 |
| (1,3677) | 1:13:A:ALA:HB2 | 1:12:A:GLY:HA3 | 16 | 0.32 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA2 | 17 | 0.32 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA3 | 17 | 0.32 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD11 | 10 | 0.32 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD12 | 10 | 0.32 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD13 | 10 | 0.32 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD21 | 10 | 0.32 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD22 | 10 | 0.32 |
| (1,3644) | 1:113:A:LEU:HD23 | 1:17:A:LEU:HD23 | 10 | 0.32 |
| (1,3620) | 1:198:A:GLY:HA2 | 1:197:A:PHE:HA | 10 | 0.32 |
| (1,3620) | 1:166:A:GLY:HA3 | 1:163:A:SER:HA | 15 | 0.32 |
| (1,3599) | 1:129:A:ILE:HG23 | 1:37:A:THR:HG21 | 19 | 0.32 |
| (1,3599) | 1:129:A:ILE:HG23 | 1:37:A:THR:HG22 | 19 | 0.32 |
| (1,3599) | 1:129:A:ILE:HG23 | 1:37:A:THR:HG23 | 19 | 0.32 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB2 | 14 | 0.32 |
| (1,3586) | 1:86:A:TYR:HB3 | 1:35:A:LEU:HB3 | 14 | 0.32 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 4 | 0.32 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 4 | 0.32 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 4 | 0.32 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 4 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 4 | 0.32 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 4 | 0.32 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB2 | 1 | 0.32 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB3 | 1 | 0.32 |
| (1,3474) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HB2 | 10 | 0.32 |
| (1,3474) | 1:67:A:ALA:HB1 | 1:69:A:PHE:HB3 | 10 | 0.32 |
| (1,3474) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HB2 | 10 | 0.32 |
| (1,3474) | 1:67:A:ALA:HB2 | 1:69:A:PHE:HB3 | 10 | 0.32 |
| (1,3474) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HB2 | 10 | 0.32 |
| (1,3474) | 1:67:A:ALA:HB3 | 1:69:A:PHE:HB3 | 10 | 0.32 |
| (1,3464) | 1:134:A:GLY:HA3 | 1:133:A:SER:HA | 19 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG2 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG3 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG2 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG3 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG2 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG3 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG2 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG3 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG2 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG3 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG2 | 8 | 0.32 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG3 | 8 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB2 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB3 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB2 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB3 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB2 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB3 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB2 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB3 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB2 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB3 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB2 | 14 | 0.32 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB3 | 14 | 0.32 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 14 | 0.32 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 17 | 0.32 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD11 | 19 | 0.32 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD12 | 19 | 0.32 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD13 | 19 | 0.32 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD21 | 19 | 0.32 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD22 | 19 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD23 | 19 | 0.32 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 8 | 0.32 |
| (1,3286) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 8 | 0.32 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 12 | 0.32 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 12 | 0.32 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 18 | 0.32 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 18 | 0.32 |
| (1,3268) | 1:9:A:ALA:HA | 1:113:A:LEU:HG | 20 | 0.32 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 1 | 0.32 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB2 | 12 | 0.32 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB3 | 12 | 0.32 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 12 | 0.32 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG21 | 5 | 0.32 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG22 | 5 | 0.32 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG23 | 5 | 0.32 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 10 | 0.32 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 10 | 0.32 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 10 | 0.32 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 10 | 0.32 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 10 | 0.32 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 10 | 0.32 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 17 | 0.32 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 17 | 0.32 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 17 | 0.32 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 17 | 0.32 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 17 | 0.32 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 17 | 0.32 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 6 | 0.32 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 9 | 0.31 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 9 | 0.31 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 8 | 0.31 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 8 | 0.31 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 8 | 0.31 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 14 | 0.31 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 18 | 0.31 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 18 | 0.31 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 18 | 0.31 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 18 | 0.31 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 18 | 0.31 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 18 | 0.31 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB2 | 12 | 0.31 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB3 | 12 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 6 | 0.31 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 6 | 0.31 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 6 | 0.31 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 6 | 0.31 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD11 | 10 | 0.31 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD12 | 10 | 0.31 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD13 | 10 | 0.31 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD21 | 10 | 0.31 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD22 | 10 | 0.31 |
| (1,3689) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HD23 | 10 | 0.31 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG11 | 6 | 0.31 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG12 | 6 | 0.31 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG13 | 6 | 0.31 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG21 | 6 | 0.31 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG22 | 6 | 0.31 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG23 | 6 | 0.31 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA2 | 3 | 0.31 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA3 | 3 | 0.31 |
| (1,3655) | 1:87:A:ALA:HB2 | 1:35:A:LEU:HA | 12 | 0.31 |
| (1,3645) | 1:25:A:LEU:HD11 | 1:180:A:SER:H | 9 | 0.31 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD11 | 20 | 0.31 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD12 | 20 | 0.31 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD13 | 20 | 0.31 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD21 | 20 | 0.31 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD22 | 20 | 0.31 |
| (1,3644) | 1:113:A:LEU:HD11 | 1:17:A:LEU:HD23 | 20 | 0.31 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB2 | 9 | 0.31 |
| (1,3639) | 1:156:A:TYR:HB2 | 1:155:A:SER:HB3 | 9 | 0.31 |
| (1,3620) | 1:198:A:GLY:HA2 | 1:197:A:PHE:HA | 17 | 0.31 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG2 | 18 | 0.31 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG3 | 18 | 0.31 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG2 | 3 | 0.31 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG3 | 3 | 0.31 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB2 | 18 | 0.31 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB3 | 18 | 0.31 |
| (1,3419) | 1:18:A:ILE:HG12 | 1:172:A:PRO:HG2 | 19 | 0.31 |
| (1,3419) | 1:18:A:ILE:HG12 | 1:172:A:PRO:HG3 | 19 | 0.31 |
| (1,3419) | 1:18:A:ILE:HG13 | 1:172:A:PRO:HG2 | 19 | 0.31 |
| (1,3419) | 1:18:A:ILE:HG13 | 1:172:A:PRO:HG3 | 19 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 14 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 14 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 14 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 14 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 14 | 0.31 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 14 | 0.31 |
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 12 | 0.31 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 13 | 0.31 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 13 | 0.31 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:129:A:ILE:HD11 | 3 | 0.31 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:129:A:ILE:HD12 | 3 | 0.31 |
| (1,3332) | 1:52:A:ALA:HB2 | 1:129:A:ILE:HD13 | 3 | 0.31 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 18 | 0.31 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 18 | 0.31 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 18 | 0.31 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 18 | 0.31 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 13 | 0.31 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 13 | 0.31 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB2 | 9 | 0.31 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB3 | 9 | 0.31 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB2 | 9 | 0.31 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB3 | 9 | 0.31 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 14 | 0.31 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 14 | 0.31 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 3 | 0.31 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 3 | 0.31 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 3 | 0.31 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 3 | 0.31 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 3 | 0.31 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 3 | 0.31 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 15 | 0.31 |
| (1,1123) | 1:132:A:ASP:H | 1:71:A:VAL:HB | 19 | 0.31 |
| (1,1095) | 1:193:A:GLY:H | 1:194:A:GLN:HA | 9 | 0.31 |
| (1,1078) | 1:56:A:ALA:H | 1:50:A:ARG:HE | 10 | 0.31 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 15 | 0.31 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 15 | 0.31 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 15 | 0.31 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 13 | 0.31 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 13 | 0.31 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 13 | 0.31 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 3 | 0.31 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 20 | 0.31 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 20 | 0.31 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 20 | 0.31 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 20 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 20 | 0.31 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 20 | 0.31 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 15 | 0.31 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 15 | 0.31 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 15 | 0.31 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 15 | 0.31 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 15 | 0.31 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 15 | 0.31 |
| (1,897) | 1:156:A:TYR:HA | 1:160:A:SER:H | 5 | 0.31 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB2 | 17 | 0.31 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB3 | 17 | 0.31 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 11 | 0.3 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 11 | 0.3 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 11 | 0.3 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 18 | 0.3 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB2 | 4 | 0.3 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB3 | 4 | 0.3 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 14 | 0.3 |
| (1,3759) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 14 | 0.3 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 8 | 0.3 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB2 | 2 | 0.3 |
| (1,3697) | 1:13:A:ALA:HB1 | 1:108:A:LEU:HB3 | 2 | 0.3 |
| (1,3683) | 1:56:A:ALA:HB1 | 1:50:A:ARG:HA | 13 | 0.3 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA2 | 8 | 0.3 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:12:A:GLY:HA3 | 8 | 0.3 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 8 | 0.3 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 8 | 0.3 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 20 | 0.3 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 20 | 0.3 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB1 | 4 | 0.3 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB2 | 4 | 0.3 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB3 | 4 | 0.3 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 19 | 0.3 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 19 | 0.3 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 19 | 0.3 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 19 | 0.3 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB2 | 6 | 0.3 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB3 | 6 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG2 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG3 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG2 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG3 | 16 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG2 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG3 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG2 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG3 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG2 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG3 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG2 | 16 | 0.3 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG3 | 16 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD11 | 1:88:A:GLN:HG2 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD11 | 1:88:A:GLN:HG3 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD12 | 1:88:A:GLN:HG2 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD12 | 1:88:A:GLN:HG3 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD13 | 1:88:A:GLN:HG2 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD13 | 1:88:A:GLN:HG3 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD21 | 1:88:A:GLN:HG2 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD21 | 1:88:A:GLN:HG3 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD22 | 1:88:A:GLN:HG2 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD22 | 1:88:A:GLN:HG3 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD23 | 1:88:A:GLN:HG2 | 8 | 0.3 |
| (1,3404) | 1:31:A:LEU:HD23 | 1:88:A:GLN:HG3 | 8 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG11 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG12 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG13 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG21 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG22 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG23 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG11 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG12 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG13 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG21 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG22 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG23 | 5 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG11 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG12 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG13 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG21 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG22 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG23 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG11 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG12 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG13 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG21 | 7 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG22 | 7 | 0.3 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG23 | 7 | 0.3 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 4 | 0.3 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 4 | 0.3 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 4 | 0.3 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD11 | 2 | 0.3 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD12 | 2 | 0.3 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD13 | 2 | 0.3 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD21 | 2 | 0.3 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD22 | 2 | 0.3 |
| (1,3220) | 1:9:A:ALA:HB2 | 1:117:A:LEU:HD23 | 2 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG21 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG22 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG23 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG21 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG22 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG23 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG21 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG22 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG23 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG21 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG22 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG23 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG21 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG22 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG23 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG21 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG22 | 14 | 0.3 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG23 | 14 | 0.3 |
| (1,2781) | 1:9:A:ALA:HA | 1:114:A:SER:HB2 | 13 | 0.3 |
| (1,2781) | 1:9:A:ALA:HA | 1:114:A:SER:HB3 | 13 | 0.3 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD21 | 11 | 0.3 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD22 | 11 | 0.3 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD21 | 11 | 0.3 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD22 | 11 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 6 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 6 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 6 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 6 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 6 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 6 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 10 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 10 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 10 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 10 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 10 | 0.3 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 10 | 0.3 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 8 | 0.3 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 8 | 0.3 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 8 | 0.3 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 8 | 0.3 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 8 | 0.3 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 8 | 0.3 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 3 | 0.3 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 12 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 18 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 18 | 0.3 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 18 | 0.3 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 11 | 0.3 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 14 | 0.3 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 14 | 0.3 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 14 | 0.3 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 2 | 0.3 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 2 | 0.3 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 2 | 0.3 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 2 | 0.3 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 2 | 0.3 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 2 | 0.3 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 3 | 0.3 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 4 | 0.3 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 14 | 0.3 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 14 | 0.3 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 14 | 0.3 |
| (1,928) | 1:178:A:GLY:HA2 | 1:187:A:GLY:H | 14 | 0.3 |
| (1,928) | 1:178:A:GLY:HA3 | 1:187:A:GLY:H | 14 | 0.3 |
| (1,781) | 1:127:A:LEU:H | 1:129:A:ILE:H | 16 | 0.3 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD21 | 1 | 0.3 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD22 | 1 | 0.3 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD21 | 12 | 0.3 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD22 | 12 | 0.3 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 19 | 0.29 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 19 | 0.29 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 19 | 0.29 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 20 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 20 | 0.29 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 20 | 0.29 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD11 | 13 | 0.29 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD12 | 13 | 0.29 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD13 | 13 | 0.29 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD21 | 13 | 0.29 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD22 | 13 | 0.29 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD23 | 13 | 0.29 |
| (1,3798) | 1:154:A:ALA:HA | 1:153:A:SER:HA | 8 | 0.29 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 19 | 0.29 |
| (1,3790) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 6 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 19 | 0.29 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 19 | 0.29 |
| (1,3735) | 1:48:A:VAL:HG22 | 1:46:A:SER:H | 14 | 0.29 |
| (1,3734) | 1:37:A:THR:HA | 1:136:A:VAL:HB | 3 | 0.29 |
| (1,3731) | 1:108:A:LEU:HA | 1:108:A:LEU:HG | 7 | 0.29 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 14 | 0.29 |
| (1,3710) | 1:49:A:GLN:HB2 | 1:55:A:LEU:HA | 18 | 0.29 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD11 | 9 | 0.29 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD12 | 9 | 0.29 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD13 | 9 | 0.29 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD21 | 9 | 0.29 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD22 | 9 | 0.29 |
| (1,3689) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HD23 | 9 | 0.29 |
| (1,3683) | 1:56:A:ALA:HB3 | 1:50:A:ARG:HA | 17 | 0.29 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 16 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 16 | 0.29 |
| (1,3620) | 1:166:A:GLY:HA2 | 1:163:A:SER:HA | 11 | 0.29 |
| (1,3583) | 1:74:A:VAL:HG21 | 1:44:A:ALA:HA | 5 | 0.29 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 13 | 0.29 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 13 | 0.29 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 13 | 0.29 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 13 | 0.29 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 13 | 0.29 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 13 | 0.29 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 12 | 0.29 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 12 | 0.29 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD11 | 4 | 0.29 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD12 | 4 | 0.29 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD13 | 4 | 0.29 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD21 | 4 | 0.29 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD22 | 4 | 0.29 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD23 | 4 | 0.29 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG2 | 16 | 0.29 |
| (1,3437) | 1:101:A:ASN:HB3 | 1:194:A:GLN:HG3 | 16 | 0.29 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 19 | 0.29 |
| (1,3292) | 1:112:A:VAL:H | 1:108:A:LEU:HG | 12 | 0.29 |
| (1,3231) | 1:34:A:VAL:HG23 | 1:36:A:ARG:HA | 7 | 0.29 |
| (1,3193) | 1:191:A:PRO:HB2 | 1:192:A:PHE:HB2 | 18 | 0.29 |
| (1,3193) | 1:191:A:PRO:HB2 | 1:192:A:PHE:HB3 | 18 | 0.29 |
| (1,3193) | 1:191:A:PRO:HB3 | 1:192:A:PHE:HB2 | 18 | 0.29 |
| (1,3193) | 1:191:A:PRO:HB3 | 1:192:A:PHE:HB3 | 18 | 0.29 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB1 | 6 | 0.29 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB2 | 6 | 0.29 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB3 | 6 | 0.29 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB1 | 6 | 0.29 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB2 | 6 | 0.29 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB3 | 6 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 20 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 20 | 0.29 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 20 | 0.29 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 11 | 0.29 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 11 | 0.29 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 18 | 0.29 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 18 | 0.29 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 18 | 0.29 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 18 | 0.29 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 18 | 0.29 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 18 | 0.29 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 6 | 0.29 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 6 | 0.29 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 8 | 0.29 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 17 | 0.29 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 20 | 0.29 |
| (1,1148) | 1:134:A:GLY:H | 1:67:A:ALA:HA | 4 | 0.29 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 3 | 0.29 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 3 | 0.29 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 3 | 0.29 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 3 | 0.29 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 3 | 0.29 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 3 | 0.29 |
| (1,1138) | 1:76:A:ARG:HB3 | 1:74:A:VAL:H | 7 | 0.29 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 15 | 0.29 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 17 | 0.29 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 16 | 0.29 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 16 | 0.29 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 16 | 0.29 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 12 | 0.29 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 12 | 0.29 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 12 | 0.29 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 12 | 0.29 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 12 | 0.29 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 12 | 0.29 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 16 | 0.29 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 15 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 11 | 0.29 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 12 | 0.29 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 20 | 0.29 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD21 | 9 | 0.29 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD22 | 9 | 0.29 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD21 | 13 | 0.29 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD22 | 13 | 0.29 |
| (1,141) | 1:29:A:SER:H | 1:32:A:ARG:HD2 | 18 | 0.29 |
| (1,141) | 1:29:A:SER:H | 1:32:A:ARG:HD3 | 18 | 0.29 |
| (1,3913) | 1:99:A:VAL:HG11 | 1:95:A:PHE:HD1 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG11 | 1:95:A:PHE:HD2 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG12 | 1:95:A:PHE:HD1 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG12 | 1:95:A:PHE:HD2 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG13 | 1:95:A:PHE:HD1 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG13 | 1:95:A:PHE:HD2 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG21 | 1:95:A:PHE:HD1 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG21 | 1:95:A:PHE:HD2 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG22 | 1:95:A:PHE:HD1 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG22 | 1:95:A:PHE:HD2 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG23 | 1:95:A:PHE:HD1 | 1 | 0.28 |
| (1,3913) | 1:99:A:VAL:HG23 | 1:95:A:PHE:HD2 | 1 | 0.28 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD11 | 1 | 0.28 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD12 | 1 | 0.28 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD13 | 1 | 0.28 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD21 | 1 | 0.28 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD22 | 1 | 0.28 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD23 | 1 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 16 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 16 | 0.28 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 16 | 0.28 |
| (1,3844) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 18 | 0.28 |
| (1,3796) | 1:124:A:ALA:HB2 | 1:120:A:VAL:HA | 1 | 0.28 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 16 | 0.28 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 4 | 0.28 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 4 | 0.28 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 18 | 0.28 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 18 | 0.28 |
| (1,3649) | 1:129:A:ILE:HG22 | 1:131:A:VAL:H | 4 | 0.28 |
| (1,3649) | 1:129:A:ILE:HG22 | 1:129:A:ILE:H | 10 | 0.28 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD11 | 4 | 0.28 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD12 | 4 | 0.28 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD13 | 4 | 0.28 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD21 | 4 | 0.28 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD22 | 4 | 0.28 |
| (1,3607) | 1:36:A:ARG:HE | 1:116:A:LEU:HD23 | 4 | 0.28 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 17 | 0.28 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 17 | 0.28 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 17 | 0.28 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 17 | 0.28 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 17 | 0.28 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 17 | 0.28 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 9 | 0.28 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 9 | 0.28 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 3 | 0.28 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB2 | 16 | 0.28 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB3 | 16 | 0.28 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 17 | 0.28 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 17 | 0.28 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 17 | 0.28 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 17 | 0.28 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB2 | 12 | 0.28 |
| (1,3286) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HB3 | 12 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 8 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 8 | 0.28 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 8 | 0.28 |
| (1,3128) | 1:170:A:THR:HA | 1:174:A:GLY:HA2 | 1 | 0.28 |
| (1,3128) | 1:170:A:THR:HA | 1:174:A:GLY:HA3 | 1 | 0.28 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD11 | 4 | 0.28 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD12 | 4 | 0.28 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD13 | 4 | 0.28 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD21 | 4 | 0.28 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD22 | 4 | 0.28 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD23 | 4 | 0.28 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 4 | 0.28 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 4 | 0.28 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 6 | 0.28 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 6 | 0.28 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 8 | 0.28 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 14 | 0.28 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 4 | 0.28 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 4 | 0.28 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 4 | 0.28 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 4 | 0.28 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 4 | 0.28 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 4 | 0.28 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD11 | 18 | 0.28 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD12 | 18 | 0.28 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD13 | 18 | 0.28 |
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE21 | 5 | 0.28 |
| (1,1078) | 1:56:A:ALA:H | 1:53:A:GLN:HE22 | 5 | 0.28 |
| (1,1065) | 1:50:A:ARG:HB3 | 1:50:A:ARG:HE | 12 | 0.28 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 19 | 0.28 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 19 | 0.28 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 19 | 0.28 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 12 | 0.28 |
| (1,1039) | 1:90:A:PHE:H | 1:18:A:ILE:HB | 8 | 0.28 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 7 | 0.28 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 1 | 0.28 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 1 | 0.28 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 14 | 0.28 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 14 | 0.28 |
| (1,999) | 1:134:A:GLY:HA2 | 1:132:A:ASP:H | 4 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,999) | 1:134:A:GLY:HA3 | 1:132:A:ASP:H | 4 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG11 | 9 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG12 | 9 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG13 | 9 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG21 | 9 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG22 | 9 | 0.28 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG23 | 9 | 0.28 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 18 | 0.28 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 11 | 0.28 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 11 | 0.28 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 7 | 0.28 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 7 | 0.28 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 14 | 0.27 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 14 | 0.27 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 14 | 0.27 |
| (1,3798) | 1:161:A:ALA:HA | 1:162:A:SER:HA | 16 | 0.27 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 3 | 0.27 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 3 | 0.27 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 3 | 0.27 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 3 | 0.27 |
| (1,3649) | 1:129:A:ILE:HG21 | 1:131:A:VAL:H | 3 | 0.27 |
| (1,3649) | 1:129:A:ILE:HG22 | 1:129:A:ILE:H | 17 | 0.27 |
| (1,3587) | 1:96:A:ASN:HB3 | 1:124:A:ALA:HB1 | 11 | 0.27 |
| (1,3587) | 1:96:A:ASN:HB3 | 1:124:A:ALA:HB2 | 11 | 0.27 |
| (1,3587) | 1:96:A:ASN:HB3 | 1:124:A:ALA:HB3 | 11 | 0.27 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 5 | 0.27 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 5 | 0.27 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 9 | 0.27 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 9 | 0.27 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB1 | 19 | 0.27 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB2 | 19 | 0.27 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB3 | 19 | 0.27 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 18 | 0.27 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 18 | 0.27 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 18 | 0.27 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 18 | 0.27 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 18 | 0.27 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 18 | 0.27 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD11 | 2 | 0.27 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD12 | 2 | 0.27 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD13 | 2 | 0.27 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD21 | 2 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD22 | 2 | 0.27 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD23 | 2 | 0.27 |
| (1,3374) | 1:93:A:ALA:HB3 | 1:90:A:PHE:HA | 2 | 0.27 |
| (1,3322) | 1:108:A:LEU:HD22 | 1:107:A:THR:HB | 8 | 0.27 |
| (1,3202) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HA | 8 | 0.27 |
| (1,3202) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 8 | 0.27 |
| (1,3202) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 8 | 0.27 |
| (1,3202) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HA | 8 | 0.27 |
| (1,3202) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HA | 8 | 0.27 |
| (1,3202) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HA | 8 | 0.27 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB2 | 4 | 0.27 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB3 | 4 | 0.27 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB2 | 4 | 0.27 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB3 | 4 | 0.27 |
| (1,2869) | 1:55:A:LEU:HB2 | 1:120:A:VAL:HA | 15 | 0.27 |
| (1,2869) | 1:55:A:LEU:HB3 | 1:120:A:VAL:HA | 15 | 0.27 |
| (1,2482) | 1:85:A:ALA:H | 1:86:A:TYR:HB2 | 10 | 0.27 |
| (1,2482) | 1:85:A:ALA:H | 1:86:A:TYR:HB3 | 10 | 0.27 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB2 | 3 | 0.27 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB3 | 3 | 0.27 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG11 | 18 | 0.27 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG12 | 18 | 0.27 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG13 | 18 | 0.27 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG21 | 18 | 0.27 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG22 | 18 | 0.27 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG23 | 18 | 0.27 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 17 | 0.27 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 17 | 0.27 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 17 | 0.27 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 19 | 0.27 |
| (1,1095) | 1:193:A:GLY:H | 1:191:A:PRO:HA | 14 | 0.27 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG21 | 7 | 0.27 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG22 | 7 | 0.27 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG23 | 7 | 0.27 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD11 | 20 | 0.27 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD12 | 20 | 0.27 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD13 | 20 | 0.27 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD21 | 20 | 0.27 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD22 | 20 | 0.27 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD23 | 20 | 0.27 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 1 | 0.27 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 2 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 13 | 0.27 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 13 | 0.27 |
| (1,1028) | 1:71:A:VAL:H | 1:72:A:GLN:HA | 20 | 0.27 |
| (1,1025) | 1:72:A:GLN:H | 1:67:A:ALA:HA | 8 | 0.27 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 2 | 0.27 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 17 | 0.27 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD11 | 15 | 0.27 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD12 | 15 | 0.27 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD13 | 15 | 0.27 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD21 | 15 | 0.27 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD22 | 15 | 0.27 |
| (1,962) | 1:117:A:LEU:H | 1:113:A:LEU:HD23 | 15 | 0.27 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 1 | 0.27 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 7 | 0.27 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 13 | 0.27 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 20 | 0.27 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 20 | 0.27 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 20 | 0.27 |
| (1,925) | 1:185:A:PRO:HG2 | 1:186:A:LEU:H | 19 | 0.27 |
| (1,925) | 1:185:A:PRO:HG3 | 1:186:A:LEU:H | 19 | 0.27 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 12 | 0.27 |
| (1,903) | 1:163:A:SER:HA | 1:166:A:GLY:H | 3 | 0.27 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB2 | 19 | 0.27 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB3 | 19 | 0.27 |
| (1,692) | 1:117:A:LEU:H | 1:117:A:LEU:HG | 13 | 0.27 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB2 | 15 | 0.27 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB3 | 15 | 0.27 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 1 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 2 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD2 | 1:95:A:PHE:HZ | 3 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 4 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 5 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 6 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 7 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 8 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD2 | 1:95:A:PHE:HZ | 9 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 10 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 12 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 13 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 14 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 15 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 16 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 17 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 18 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 19 | 0.26 |
| (1,3912) | 1:95:A:PHE:HD1 | 1:95:A:PHE:HZ | 20 | 0.26 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 13 | 0.26 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 13 | 0.26 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 5 | 0.26 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 5 | 0.26 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 11 | 0.26 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 11 | 0.26 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 8 | 0.26 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 8 | 0.26 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 8 | 0.26 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 8 | 0.26 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 8 | 0.26 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 8 | 0.26 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 3 | 0.26 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 3 | 0.26 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 3 | 0.26 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB2 | 4 | 0.26 |
| (1,3849) | 1:51:A:ALA:HB2 | 1:132:A:ASP:HB3 | 4 | 0.26 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 2 | 0.26 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 2 | 0.26 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 2 | 0.26 |
| (1,3796) | 1:124:A:ALA:HB2 | 1:120:A:VAL:HA | 18 | 0.26 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB2 | 4 | 0.26 |
| (1,3760) | 1:85:A:ALA:HA | 1:86:A:TYR:HB3 | 4 | 0.26 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG21 | 12 | 0.26 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG22 | 12 | 0.26 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG23 | 12 | 0.26 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 4 | 0.26 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB2 | 9 | 0.26 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB3 | 9 | 0.26 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:14:A:SER:HB2 | 5 | 0.26 |
| (1,3677) | 1:13:A:ALA:HB3 | 1:14:A:SER:HB3 | 5 | 0.26 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB2 | 12 | 0.26 |
| (1,3677) | 1:13:A:ALA:HB1 | 1:14:A:SER:HB3 | 12 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3639) | 1:156:A:TYR:HB3 | 1:155:A:SER:HB2 | 13 | 0.26 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:155:A:SER:HB3 | 13 | 0.26 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE1 | 5 | 0.26 |
| (1,3623) | 1:140:A:ILE:HD11 | 1:95:A:PHE:HE2 | 5 | 0.26 |
| (1,3620) | 1:193:A:GLY:HA2 | 1:192:A:PHE:HA | 13 | 0.26 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE21 | 15 | 0.26 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE22 | 15 | 0.26 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE21 | 19 | 0.26 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE22 | 19 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB1 | 13 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB2 | 13 | 0.26 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB3 | 13 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG23 | 1:73:A:ALA:HB1 | 14 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG23 | 1:73:A:ALA:HB2 | 14 | 0.26 |
| (1,3500) | 1:74:A:VAL:HG23 | 1:73:A:ALA:HB3 | 14 | 0.26 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 13 | 0.26 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 13 | 0.26 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 13 | 0.26 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 13 | 0.26 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 13 | 0.26 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 13 | 0.26 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD11 | 1 | 0.26 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD12 | 1 | 0.26 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD13 | 1 | 0.26 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD21 | 1 | 0.26 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD22 | 1 | 0.26 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD23 | 1 | 0.26 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 2 | 0.26 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 6 | 0.26 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 9 | 0.26 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 20 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG11 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG12 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG13 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG21 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG22 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG23 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG11 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG12 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG13 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG21 | 2 | 0.26 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG22 | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG23 | 2 | 0.26 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB2 | 1 | 0.26 |
| (1,3336) | 1:21:A:VAL:HB | 1:191:A:PRO:HB3 | 1 | 0.26 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB2 | 4 | 0.26 |
| (1,3295) | 1:39:A:VAL:HG23 | 1:36:A:ARG:HB3 | 4 | 0.26 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 9 | 0.26 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 9 | 0.26 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 9 | 0.26 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 9 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB2 | 1:74:A:VAL:HG11 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB2 | 1:74:A:VAL:HG12 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB2 | 1:74:A:VAL:HG13 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB2 | 1:74:A:VAL:HG21 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB2 | 1:74:A:VAL:HG22 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB2 | 1:74:A:VAL:HG23 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB3 | 1:74:A:VAL:HG11 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB3 | 1:74:A:VAL:HG12 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB3 | 1:74:A:VAL:HG13 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB3 | 1:74:A:VAL:HG21 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB3 | 1:74:A:VAL:HG22 | 5 | 0.26 |
| (1,3281) | 1:77:A:LEU:HB3 | 1:74:A:VAL:HG23 | 5 | 0.26 |
| (1,3088) | 1:148:A:SER:HB2 | 1:149:A:THR:HG21 | 9 | 0.26 |
| (1,3088) | 1:148:A:SER:HB2 | 1:149:A:THR:HG22 | 9 | 0.26 |
| (1,3088) | 1:148:A:SER:HB2 | 1:149:A:THR:HG23 | 9 | 0.26 |
| (1,3088) | 1:148:A:SER:HB3 | 1:149:A:THR:HG21 | 9 | 0.26 |
| (1,3088) | 1:148:A:SER:HB3 | 1:149:A:THR:HG22 | 9 | 0.26 |
| (1,3088) | 1:148:A:SER:HB3 | 1:149:A:THR:HG23 | 9 | 0.26 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 18 | 0.26 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 18 | 0.26 |
| (1,2097) | 1:43:A:ILE:HD11 | 1:44:A:ALA:HA | 20 | 0.26 |
| (1,2097) | 1:43:A:ILE:HD12 | 1:44:A:ALA:HA | 20 | 0.26 |
| (1,2097) | 1:43:A:ILE:HD13 | 1:44:A:ALA:HA | 20 | 0.26 |
| (1,1958) | 1:30:A:THR:HB | 1:31:A:LEU:H | 14 | 0.26 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 3 | 0.26 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 18 | 0.26 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 18 | 0.26 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG11 | 7 | 0.26 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG12 | 7 | 0.26 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG13 | 7 | 0.26 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG21 | 7 | 0.26 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG22 | 7 | 0.26 |
| (1,1162) | 1:46:A:SER:H | 1:47:A:VAL:HG23 | 7 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG11 | 7 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG12 | 7 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG13 | 7 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG21 | 7 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG22 | 7 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:48:A:VAL:HG23 | 7 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 20 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 20 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 20 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 20 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 20 | 0.26 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 20 | 0.26 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 1 | 0.26 |
| (1,1138) | 1:147:A:LEU:HB3 | 1:149:A:THR:H | 14 | 0.26 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 14 | 0.26 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD11 | 17 | 0.26 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD12 | 17 | 0.26 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD13 | 17 | 0.26 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD21 | 17 | 0.26 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD22 | 17 | 0.26 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD23 | 17 | 0.26 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG11 | 12 | 0.26 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG12 | 12 | 0.26 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG13 | 12 | 0.26 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG21 | 12 | 0.26 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG22 | 12 | 0.26 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG23 | 12 | 0.26 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 4 | 0.26 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 10 | 0.26 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 18 | 0.26 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 18 | 0.26 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 18 | 0.26 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 18 | 0.26 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 18 | 0.26 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 18 | 0.26 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 10 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 3 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 3 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 7 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 7 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 11 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 18 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 18 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 19 | 0.26 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 19 | 0.26 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG11 | 14 | 0.26 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG12 | 14 | 0.26 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG13 | 14 | 0.26 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG21 | 14 | 0.26 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG22 | 14 | 0.26 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG23 | 14 | 0.26 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA2 | 20 | 0.26 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA3 | 20 | 0.26 |
| (1,892) | 1:153:A:SER:H | 1:158:A:GLN:HB2 | 15 | 0.26 |
| (1,892) | 1:153:A:SER:H | 1:158:A:GLN:HB3 | 15 | 0.26 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 3 | 0.26 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB2 | 18 | 0.26 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB3 | 18 | 0.26 |
| (1,299) | 1:49:A:GLN:H | 1:58:A:THR:HB | 17 | 0.26 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 1 | 0.25 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 1 | 0.25 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 18 | 0.25 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 18 | 0.25 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 18 | 0.25 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 18 | 0.25 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 18 | 0.25 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 18 | 0.25 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD11 | 12 | 0.25 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD12 | 12 | 0.25 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD13 | 12 | 0.25 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD21 | 12 | 0.25 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD22 | 12 | 0.25 |
| (1,3863) | 1:129:A:ILE:HG12 | 1:55:A:LEU:HD23 | 12 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 2 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 2 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 14 | 0.25 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 14 | 0.25 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB2 | 19 | 0.25 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB3 | 19 | 0.25 |
| (1,3683) | 1:56:A:ALA:HB3 | 1:50:A:ARG:HA | 19 | 0.25 |
| (1,3655) | 1:87:A:ALA:HB3 | 1:39:A:VAL:HA | 5 | 0.25 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB2 | 12 | 0.25 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB3 | 12 | 0.25 |
| (1,3649) | 1:129:A:ILE:HG22 | 1:131:A:VAL:H | 7 | 0.25 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 6 | 0.25 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 6 | 0.25 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 14 | 0.25 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 14 | 0.25 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 14 | 0.25 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 14 | 0.25 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 14 | 0.25 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 14 | 0.25 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA2 | 20 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA3 | 20 | 0.25 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 20 | 0.25 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 20 | 0.25 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD11 | 2 | 0.25 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD12 | 2 | 0.25 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD13 | 2 | 0.25 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD21 | 2 | 0.25 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD22 | 2 | 0.25 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD23 | 2 | 0.25 |
| (1,3476) | 1:56:A:ALA:HB1 | 1:48:A:VAL:HA | 17 | 0.25 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD11 | 9 | 0.25 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD12 | 9 | 0.25 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD13 | 9 | 0.25 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD21 | 9 | 0.25 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD22 | 9 | 0.25 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD23 | 9 | 0.25 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 16 | 0.25 |
| (1,3455) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 16 | 0.25 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:132:A:ASP:HB2 | 3 | 0.25 |
| (1,3422) | 1:35:A:LEU:HD12 | 1:132:A:ASP:HB3 | 3 | 0.25 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD2 | 17 | 0.25 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD3 | 17 | 0.25 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD2 | 17 | 0.25 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD3 | 17 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB2 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB3 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB2 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB3 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB2 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB3 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB2 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB3 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB2 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB3 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB2 | 3 | 0.25 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB3 | 3 | 0.25 |
| (1,3400) | 1:140:A:ILE:HD11 | 1:141:A:SER:HB2 | 17 | 0.25 |
| (1,3400) | 1:140:A:ILE:HD11 | 1:141:A:SER:HB3 | 17 | 0.25 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 1 | 0.25 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 15 | 0.25 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 15 | 0.25 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD11 | 18 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD12 | 18 | 0.25 |
| (1,3332) | 1:52:A:ALA:HB3 | 1:129:A:ILE:HD13 | 18 | 0.25 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD11 | 12 | 0.25 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD12 | 12 | 0.25 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD13 | 12 | 0.25 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD21 | 12 | 0.25 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD22 | 12 | 0.25 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD23 | 12 | 0.25 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB2 | 5 | 0.25 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB3 | 5 | 0.25 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB2 | 13 | 0.25 |
| (1,3295) | 1:10:A:THR:HG22 | 1:42:A:GLN:HB3 | 13 | 0.25 |
| (1,3295) | 1:10:A:THR:HG23 | 1:42:A:GLN:HB2 | 16 | 0.25 |
| (1,3295) | 1:10:A:THR:HG23 | 1:42:A:GLN:HB3 | 16 | 0.25 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB2 | 20 | 0.25 |
| (1,3295) | 1:10:A:THR:HG21 | 1:42:A:GLN:HB3 | 20 | 0.25 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 11 | 0.25 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 11 | 0.25 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 11 | 0.25 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 11 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 1 | 0.25 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 1 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD11 | 10 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD12 | 10 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD13 | 10 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD21 | 10 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD22 | 10 | 0.25 |
| (1,3214) | 1:14:A:SER:HB3 | 1:100:A:LEU:HD23 | 10 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA2 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA3 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA2 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA3 | 17 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA2 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA3 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA2 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA3 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA2 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA3 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA2 | 17 | 0.25 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA3 | 17 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG21 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG22 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD11 | 1:149:A:THR:HG23 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG21 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG22 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD12 | 1:149:A:THR:HG23 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG21 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG22 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD13 | 1:149:A:THR:HG23 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG21 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG22 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD21 | 1:149:A:THR:HG23 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG21 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG22 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD22 | 1:149:A:THR:HG23 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG21 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG22 | 5 | 0.25 |
| (1,3091) | 1:25:A:LEU:HD23 | 1:149:A:THR:HG23 | 5 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 10 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 10 | 0.25 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 10 | 0.25 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 7 | 0.25 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 7 | 0.25 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD11 | 15 | 0.25 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD12 | 15 | 0.25 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD13 | 15 | 0.25 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD21 | 15 | 0.25 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD22 | 15 | 0.25 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD23 | 15 | 0.25 |
| (1,2112) | 1:41:A:GLN:HE21 | 1:45:A:SER:HA | 6 | 0.25 |
| (1,2112) | 1:41:A:GLN:HE22 | 1:45:A:SER:HA | 6 | 0.25 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 4 | 0.25 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 13 | 0.25 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 13 | 0.25 |
| (1,1113) | 1:65:A:ASN:HD21 | 1:47:A:VAL:HB | 5 | 0.25 |
| (1,1107) | 1:109:A:GLY:H | 1:112:A:VAL:HB | 15 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 4 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 4 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 4 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 8 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 8 | 0.25 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 8 | 0.25 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 6 | 0.25 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 6 | 0.25 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 6 | 0.25 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD11 | 10 | 0.25 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD12 | 10 | 0.25 |
| (1,1045) | 1:45:A:SER:H | 1:43:A:ILE:HD13 | 10 | 0.25 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 19 | 0.25 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 5 | 0.25 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 5 | 0.25 |
| (1,989) | 1:110:A:SER:H | 1:108:A:LEU:HG | 15 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 4 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 4 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 4 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 4 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 4 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 4 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 20 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 20 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 20 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 20 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 20 | 0.25 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 20 | 0.25 |
| (1,927) | 1:179:A:PRO:HD2 | 1:187:A:GLY:H | 17 | 0.25 |
| (1,927) | 1:179:A:PRO:HD3 | 1:187:A:GLY:H | 17 | 0.25 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 3 | 0.25 |
| (1,917) | 1:161:A:ALA:H | 1:177:A:THR:HB | 20 | 0.25 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD2 | 9 | 0.25 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD3 | 9 | 0.25 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB2 | 14 | 0.25 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB3 | 14 | 0.25 |
| (1,3791) | 1:44:A:ALA:HB1 | 1:74:A:VAL:HA | 3 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG2 | 11 | 0.24 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG3 | 11 | 0.24 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 18 | 0.24 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 7 | 0.24 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 7 | 0.24 |
| (1,3645) | 1:94:A:LEU:HD11 | 1:40:A:SER:H | 17 | 0.24 |
| (1,3617) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HB2 | 2 | 0.24 |
| (1,3617) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HB3 | 2 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 7 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 7 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 7 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 7 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 7 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 7 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 20 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 20 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 20 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 20 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 20 | 0.24 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 20 | 0.24 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB1 | 19 | 0.24 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB2 | 19 | 0.24 |
| (1,3587) | 1:96:A:ASN:HB2 | 1:124:A:ALA:HB3 | 19 | 0.24 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA2 | 16 | 0.24 |
| (1,3572) | 1:85:A:ALA:HB3 | 1:80:A:GLY:HA3 | 16 | 0.24 |
| (1,3497) | 1:90:A:PHE:HA | 1:92:A:SER:HB2 | 10 | 0.24 |
| (1,3497) | 1:90:A:PHE:HA | 1:92:A:SER:HB3 | 10 | 0.24 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD11 | 16 | 0.24 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD12 | 16 | 0.24 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD13 | 16 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD21 | 16 | 0.24 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD22 | 16 | 0.24 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD23 | 16 | 0.24 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB2 | 20 | 0.24 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB3 | 20 | 0.24 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB2 | 20 | 0.24 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB3 | 20 | 0.24 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD11 | 11 | 0.24 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD12 | 11 | 0.24 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD13 | 11 | 0.24 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD21 | 11 | 0.24 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD22 | 11 | 0.24 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD23 | 11 | 0.24 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB2 | 12 | 0.24 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB3 | 12 | 0.24 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD2 | 17 | 0.24 |
| (1,3381) | 1:177:A:THR:HG23 | 1:179:A:PRO:HD3 | 17 | 0.24 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 14 | 0.24 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 14 | 0.24 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 14 | 0.24 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 14 | 0.24 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 20 | 0.24 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 20 | 0.24 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 18 | 0.24 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 18 | 0.24 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 18 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD2 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD3 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD2 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD3 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD2 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD3 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD2 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD3 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD2 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD3 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD2 | 19 | 0.24 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD3 | 19 | 0.24 |
| (1,3168) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HB1 | 19 | 0.24 |
| (1,3168) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HB2 | 19 | 0.24 |
| (1,3168) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HB3 | 19 | 0.24 |
| (1,3168) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HB1 | 19 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3168) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HB2 | 19 | 0.24 |
| (1,3168) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HB3 | 19 | 0.24 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 5 | 0.24 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 5 | 0.24 |
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 5 | 0.24 |
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 5 | 0.24 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB2 | 5 | 0.24 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB3 | 5 | 0.24 |
| (1,3087) | 1:148:A:SER:HB2 | 1:149:A:THR:HB | 11 | 0.24 |
| (1,3087) | 1:148:A:SER:HB3 | 1:149:A:THR:HB | 11 | 0.24 |
| (1,2970) | 1:37:A:THR:HA | 1:131:A:VAL:HB | 9 | 0.24 |
| (1,2558) | 1:21:A:VAL:HG11 | 1:93:A:ALA:HA | 5 | 0.24 |
| (1,2558) | 1:21:A:VAL:HG12 | 1:93:A:ALA:HA | 5 | 0.24 |
| (1,2558) | 1:21:A:VAL:HG13 | 1:93:A:ALA:HA | 5 | 0.24 |
| (1,2558) | 1:21:A:VAL:HG21 | 1:93:A:ALA:HA | 5 | 0.24 |
| (1,2558) | 1:21:A:VAL:HG22 | 1:93:A:ALA:HA | 5 | 0.24 |
| (1,2558) | 1:21:A:VAL:HG23 | 1:93:A:ALA:HA | 5 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG21 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG22 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG23 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG21 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG22 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG23 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG21 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG22 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG23 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG21 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG22 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG23 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG21 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG22 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG23 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG21 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG22 | 10 | 0.24 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG23 | 10 | 0.24 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 13 | 0.24 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 13 | 0.24 |
| (1,2112) | 1:41:A:GLN:HE21 | 1:45:A:SER:HA | 15 | 0.24 |
| (1,2112) | 1:41:A:GLN:HE22 | 1:45:A:SER:HA | 15 | 0.24 |
| (1,2094) | 1:1:A:ALA:HB1 | 1:43:A:ILE:HA | 9 | 0.24 |
| (1,2094) | 1:1:A:ALA:HB2 | 1:43:A:ILE:HA | 9 | 0.24 |
| (1,2094) | 1:1:A:ALA:HB3 | 1:43:A:ILE:HA | 9 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 17 | 0.24 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 17 | 0.24 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 17 | 0.24 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 17 | 0.24 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 17 | 0.24 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 17 | 0.24 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 8 | 0.24 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 10 | 0.24 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 10 | 0.24 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 10 | 0.24 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 18 | 0.24 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 18 | 0.24 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 18 | 0.24 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 11 | 0.24 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 11 | 0.24 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 11 | 0.24 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 11 | 0.24 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 11 | 0.24 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 11 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 15 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 15 | 0.24 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 15 | 0.24 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG11 | 16 | 0.24 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG12 | 16 | 0.24 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG13 | 16 | 0.24 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG21 | 16 | 0.24 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG22 | 16 | 0.24 |
| (1,1045) | 1:45:A:SER:H | 1:48:A:VAL:HG23 | 16 | 0.24 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 7 | 0.24 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 13 | 0.24 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB1 | 12 | 0.24 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB2 | 12 | 0.24 |
| (1,1013) | 1:128:A:GLY:H | 1:123:A:ALA:HB3 | 12 | 0.24 |
| (1,925) | 1:185:A:PRO:HG2 | 1:186:A:LEU:H | 11 | 0.24 |
| (1,925) | 1:185:A:PRO:HG3 | 1:186:A:LEU:H | 11 | 0.24 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 2 | 0.24 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 2 | 0.24 |
| (1,807) | 1:133:A:SER:H | 1:134:A:GLY:H | 19 | 0.24 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 20 | 0.24 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD21 | 8 | 0.24 |
| (1,326) | 1:64:A:ASN:H | 1:64:A:ASN:HD22 | 8 | 0.24 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 5 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 5 | 0.23 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 5 | 0.23 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 5 | 0.23 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 5 | 0.23 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 5 | 0.23 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 7 | 0.23 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 7 | 0.23 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 7 | 0.23 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 7 | 0.23 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 7 | 0.23 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 7 | 0.23 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 10 | 0.23 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 10 | 0.23 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 10 | 0.23 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 10 | 0.23 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 10 | 0.23 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 10 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD11 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD12 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD13 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD21 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD22 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB1 | 1:77:A:LEU:HD23 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD11 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD12 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD13 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD21 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD22 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB2 | 1:77:A:LEU:HD23 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD11 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD12 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD13 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD21 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD22 | 15 | 0.23 |
| (1,3854) | 1:79:A:ALA:HB3 | 1:77:A:LEU:HD23 | 15 | 0.23 |
| (1,3771) | 1:29:A:SER:HB2 | 1:30:A:THR:HG21 | 14 | 0.23 |
| (1,3771) | 1:29:A:SER:HB2 | 1:30:A:THR:HG22 | 14 | 0.23 |
| (1,3771) | 1:29:A:SER:HB2 | 1:30:A:THR:HG23 | 14 | 0.23 |
| (1,3771) | 1:29:A:SER:HB3 | 1:30:A:THR:HG21 | 14 | 0.23 |
| (1,3771) | 1:29:A:SER:HB3 | 1:30:A:THR:HG22 | 14 | 0.23 |
| (1,3771) | 1:29:A:SER:HB3 | 1:30:A:THR:HG23 | 14 | 0.23 |
| (1,3735) | 1:48:A:VAL:HG21 | 1:46:A:SER:H | 10 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 5 | 0.23 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG21 | 17 | 0.23 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG22 | 17 | 0.23 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG23 | 17 | 0.23 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB2 | 12 | 0.23 |
| (1,3696) | 1:129:A:ILE:HG22 | 1:50:A:ARG:HB3 | 12 | 0.23 |
| (1,3683) | 1:56:A:ALA:HB1 | 1:50:A:ARG:HA | 5 | 0.23 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD11 | 17 | 0.23 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD12 | 17 | 0.23 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD13 | 17 | 0.23 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD21 | 17 | 0.23 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD22 | 17 | 0.23 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD23 | 17 | 0.23 |
| (1,3657) | 1:77:A:LEU:HD13 | 1:73:A:ALA:HA | 10 | 0.23 |
| (1,3655) | 1:87:A:ALA:HB1 | 1:35:A:LEU:HA | 3 | 0.23 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB2 | 5 | 0.23 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB3 | 5 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 5 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 5 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 5 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 5 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 5 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 5 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 12 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 12 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 12 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 12 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 12 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 12 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 19 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 19 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 19 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 19 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 19 | 0.23 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 19 | 0.23 |
| (1,3509) | 1:170:A:THR:HA | 1:170:A:THR:HB | 1 | 0.23 |
| (1,3509) | 1:10:A:THR:HA | 1:10:A:THR:HB | 3 | 0.23 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 4 | 0.23 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 4 | 0.23 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 4 | 0.23 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 4 | 0.23 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 4 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 4 | 0.23 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB2 | 7 | 0.23 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB3 | 7 | 0.23 |
| (1,3419) | 1:18:A:ILE:HG12 | 1:172:A:PRO:HG2 | 3 | 0.23 |
| (1,3419) | 1:18:A:ILE:HG12 | 1:172:A:PRO:HG3 | 3 | 0.23 |
| (1,3419) | 1:18:A:ILE:HG13 | 1:172:A:PRO:HG2 | 3 | 0.23 |
| (1,3419) | 1:18:A:ILE:HG13 | 1:172:A:PRO:HG3 | 3 | 0.23 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 3 | 0.23 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 3 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG11 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG12 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG13 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG21 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG22 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB2 | 1:136:A:VAL:HG23 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG11 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG12 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG13 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG21 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG22 | 17 | 0.23 |
| (1,3376) | 1:130:A:ASN:HB3 | 1:136:A:VAL:HG23 | 17 | 0.23 |
| (1,3334) | 1:25:A:LEU:HA | 1:190:A:ALA:HA | 14 | 0.23 |
| (1,3268) | 1:9:A:ALA:HA | 1:113:A:LEU:HG | 6 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD11 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD12 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD13 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD21 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD22 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD23 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD11 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD12 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD13 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD21 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD22 | 5 | 0.23 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD23 | 5 | 0.23 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB2 | 17 | 0.23 |
| (1,3150) | 1:182:A:TYR:HB2 | 1:183:A:PRO:HB3 | 17 | 0.23 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB2 | 17 | 0.23 |
| (1,3150) | 1:182:A:TYR:HB3 | 1:183:A:PRO:HB3 | 17 | 0.23 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB1 | 8 | 0.23 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB2 | 8 | 0.23 |
| (1,3110) | 1:156:A:TYR:HB2 | 1:159:A:ALA:HB3 | 8 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB1 | 8 | 0.23 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB2 | 8 | 0.23 |
| (1,3110) | 1:156:A:TYR:HB3 | 1:159:A:ALA:HB3 | 8 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG21 | 3 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG22 | 3 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG23 | 3 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG21 | 3 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG22 | 3 | 0.23 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG23 | 3 | 0.23 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB2 | 5 | 0.23 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB3 | 5 | 0.23 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB2 | 5 | 0.23 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB3 | 5 | 0.23 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA2 | 7 | 0.23 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA3 | 7 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 20 | 0.23 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 20 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB2 | 7 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB3 | 7 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB2 | 7 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB3 | 7 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB2 | 17 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB3 | 17 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB2 | 17 | 0.23 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB3 | 17 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB2 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB3 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB2 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB3 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB2 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB3 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB2 | 2 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB3 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB2 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB3 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB2 | 2 | 0.23 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB3 | 2 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD1 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD2 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD1 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD2 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD1 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD2 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD1 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD2 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD1 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD2 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD1 | 3 | 0.23 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD2 | 3 | 0.23 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 20 | 0.23 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 20 | 0.23 |
| (1,1945) | 1:29:A:SER:HB2 | 1:30:A:THR:HG21 | 14 | 0.23 |
| (1,1945) | 1:29:A:SER:HB2 | 1:30:A:THR:HG22 | 14 | 0.23 |
| (1,1945) | 1:29:A:SER:HB2 | 1:30:A:THR:HG23 | 14 | 0.23 |
| (1,1945) | 1:29:A:SER:HB3 | 1:30:A:THR:HG21 | 14 | 0.23 |
| (1,1945) | 1:29:A:SER:HB3 | 1:30:A:THR:HG22 | 14 | 0.23 |
| (1,1945) | 1:29:A:SER:HB3 | 1:30:A:THR:HG23 | 14 | 0.23 |
| (1,1904) | 1:20:A:ARG:HA | 1:24:A:ALA:HA | 17 | 0.23 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB2 | 1 | 0.23 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB3 | 1 | 0.23 |
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB2 | 1 | 0.23 |
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB3 | 1 | 0.23 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 16 | 0.23 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 11 | 0.23 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 11 | 0.23 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 11 | 0.23 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 11 | 0.23 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 11 | 0.23 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 11 | 0.23 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 16 | 0.23 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 16 | 0.23 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 16 | 0.23 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 15 | 0.23 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 2 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1065) | 1:111:A:ARG:HB2 | 1:111:A:ARG:HE | 16 | 0.23 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 1 | 0.23 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 1 | 0.23 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 1 | 0.23 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 4 | 0.23 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 16 | 0.23 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 16 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD11 | 6 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD12 | 6 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD13 | 6 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD21 | 6 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD22 | 6 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD23 | 6 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD11 | 16 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD12 | 16 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD13 | 16 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD21 | 16 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD22 | 16 | 0.23 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD23 | 16 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 12 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 12 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 12 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 12 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 12 | 0.23 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 12 | 0.23 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG11 | 5 | 0.23 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG12 | 5 | 0.23 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG13 | 5 | 0.23 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG21 | 5 | 0.23 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG22 | 5 | 0.23 |
| (1,962) | 1:117:A:LEU:H | 1:120:A:VAL:HG23 | 5 | 0.23 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 20 | 0.23 |
| (1,610) | 1:101:A:ASN:HD21 | 1:105:A:ILE:H | 2 | 0.23 |
| (1,610) | 1:101:A:ASN:HD22 | 1:105:A:ILE:H | 2 | 0.23 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB2 | 2 | 0.23 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB3 | 2 | 0.23 |
| (1,141) | 1:29:A:SER:H | 1:32:A:ARG:HD2 | 17 | 0.23 |
| (1,141) | 1:29:A:SER:H | 1:32:A:ARG:HD3 | 17 | 0.23 |
| (1,3844) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 12 | 0.22 |
| (1,3791) | 1:44:A:ALA:HB2 | 1:74:A:VAL:HA | 14 | 0.22 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 17 | 0.22 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 17 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 17 | 0.22 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 17 | 0.22 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 18 | 0.22 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 18 | 0.22 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 18 | 0.22 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 18 | 0.22 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB2 | 3 | 0.22 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB3 | 3 | 0.22 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD11 | 2 | 0.22 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD12 | 2 | 0.22 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD13 | 2 | 0.22 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD21 | 2 | 0.22 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD22 | 2 | 0.22 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD23 | 2 | 0.22 |
| (1,3657) | 1:77:A:LEU:HD13 | 1:73:A:ALA:HA | 7 | 0.22 |
| (1,3654) | 1:39:A:VAL:HG13 | 1:38:A:GLY:HA2 | 2 | 0.22 |
| (1,3654) | 1:39:A:VAL:HG13 | 1:38:A:GLY:HA3 | 2 | 0.22 |
| (1,3604) | 1:57:A:SER:HA | 1:53:A:GLN:HB2 | 19 | 0.22 |
| (1,3604) | 1:57:A:SER:HA | 1:53:A:GLN:HB3 | 19 | 0.22 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 18 | 0.22 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 18 | 0.22 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 18 | 0.22 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 18 | 0.22 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 18 | 0.22 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 18 | 0.22 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG2 | 3 | 0.22 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG3 | 3 | 0.22 |
| (1,3509) | 1:170:A:THR:HA | 1:170:A:THR:HB | 17 | 0.22 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB1 | 20 | 0.22 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB2 | 20 | 0.22 |
| (1,3500) | 1:74:A:VAL:HG21 | 1:73:A:ALA:HB3 | 20 | 0.22 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 8 | 0.22 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 8 | 0.22 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 8 | 0.22 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 8 | 0.22 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 8 | 0.22 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 8 | 0.22 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 2 | 0.22 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 2 | 0.22 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 19 | 0.22 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 19 | 0.22 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 19 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3353) | 1:119:A:GLY:HA3 | 1:117:A:LEU:HA | 13 | 0.22 |
| (1,3322) | 1:108:A:LEU:HD22 | 1:107:A:THR:HB | 4 | 0.22 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 15 | 0.22 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 15 | 0.22 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB1 | 20 | 0.22 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB2 | 20 | 0.22 |
| (1,3251) | 1:47:A:VAL:HB | 1:73:A:ALA:HB3 | 20 | 0.22 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB2 | 11 | 0.22 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB3 | 11 | 0.22 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB2 | 11 | 0.22 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB3 | 11 | 0.22 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB2 | 11 | 0.22 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB3 | 11 | 0.22 |
| (1,3170) | 1:185:A:PRO:HB2 | 1:190:A:ALA:HB1 | 3 | 0.22 |
| (1,3170) | 1:185:A:PRO:HB2 | 1:190:A:ALA:HB2 | 3 | 0.22 |
| (1,3170) | 1:185:A:PRO:HB2 | 1:190:A:ALA:HB3 | 3 | 0.22 |
| (1,3170) | 1:185:A:PRO:HB3 | 1:190:A:ALA:HB1 | 3 | 0.22 |
| (1,3170) | 1:185:A:PRO:HB3 | 1:190:A:ALA:HB2 | 3 | 0.22 |
| (1,3170) | 1:185:A:PRO:HB3 | 1:190:A:ALA:HB3 | 3 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 4 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 4 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 4 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 4 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 5 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 5 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 5 | 0.22 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 5 | 0.22 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 9 | 0.22 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 9 | 0.22 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 9 | 0.22 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 9 | 0.22 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 9 | 0.22 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 9 | 0.22 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 11 | 0.22 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 11 | 0.22 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 11 | 0.22 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 15 | 0.22 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 15 | 0.22 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 5 | 0.22 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 5 | 0.22 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 14 | 0.22 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 14 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 2 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 13 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 13 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 13 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 13 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 13 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 13 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 16 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 16 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 16 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 16 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 16 | 0.22 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 16 | 0.22 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 3 | 0.22 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 9 | 0.22 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 9 | 0.22 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 9 | 0.22 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 9 | 0.22 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 10 | 0.22 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 19 | 0.22 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 16 | 0.22 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 16 | 0.22 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 16 | 0.22 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD11 | 5 | 0.22 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD12 | 5 | 0.22 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD13 | 5 | 0.22 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD21 | 5 | 0.22 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD22 | 5 | 0.22 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD23 | 5 | 0.22 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 5 | 0.22 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 15 | 0.22 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 20 | 0.22 |
| (1,1031) | 1:170:A:THR:HA | 1:169:A:TYR:H | 16 | 0.22 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 18 | 0.22 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 15 | 0.22 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 15 | 0.22 |
| (1,999) | 1:134:A:GLY:HA2 | 1:132:A:ASP:H | 15 | 0.22 |
| (1,999) | 1:134:A:GLY:HA3 | 1:132:A:ASP:H | 15 | 0.22 |
| (1,961) | 1:10:A:THR:H | 1:117:A:LEU:H | 13 | 0.22 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 14 | 0.22 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 2 | 0.22 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 2 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 6 | 0.22 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 6 | 0.22 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 16 | 0.22 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 16 | 0.22 |
| (1,875) | 1:148:A:SER:HB2 | 1:149:A:THR:H | 9 | 0.22 |
| (1,875) | 1:148:A:SER:HB3 | 1:149:A:THR:H | 9 | 0.22 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 8 | 0.22 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 8 | 0.22 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 14 | 0.22 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG11 | 18 | 0.22 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG12 | 18 | 0.22 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG13 | 18 | 0.22 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG21 | 18 | 0.22 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG22 | 18 | 0.22 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG23 | 18 | 0.22 |
| (1,236) | 1:47:A:VAL:HG11 | 1:48:A:VAL:H | 5 | 0.22 |
| (1,236) | 1:47:A:VAL:HG12 | 1:48:A:VAL:H | 5 | 0.22 |
| (1,236) | 1:47:A:VAL:HG13 | 1:48:A:VAL:H | 5 | 0.22 |
| (1,236) | 1:47:A:VAL:HG21 | 1:48:A:VAL:H | 5 | 0.22 |
| (1,236) | 1:47:A:VAL:HG22 | 1:48:A:VAL:H | 5 | 0.22 |
| (1,236) | 1:47:A:VAL:HG23 | 1:48:A:VAL:H | 5 | 0.22 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 8 | 0.21 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 8 | 0.21 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 9 | 0.21 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 9 | 0.21 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 9 | 0.21 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 9 | 0.21 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 9 | 0.21 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 9 | 0.21 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD1 | 19 | 0.21 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD2 | 19 | 0.21 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD1 | 19 | 0.21 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD2 | 19 | 0.21 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD1 | 19 | 0.21 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD2 | 19 | 0.21 |
| (1,3849) | 1:51:A:ALA:HB3 | 1:132:A:ASP:HB2 | 1 | 0.21 |
| (1,3849) | 1:51:A:ALA:HB3 | 1:132:A:ASP:HB3 | 1 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 14 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 14 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 14 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 14 | 0.21 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 14 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 14 | 0.21 |
| (1,3756) | 1:156:A:TYR:HB2 | 1:157:A:SER:HA | 1 | 0.21 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 18 | 0.21 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 18 | 0.21 |
| (1,3683) | 1:56:A:ALA:HB1 | 1:50:A:ARG:HA | 12 | 0.21 |
| (1,3683) | 1:56:A:ALA:HB2 | 1:50:A:ARG:HA | 16 | 0.21 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 5 | 0.21 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 5 | 0.21 |
| (1,3657) | 1:77:A:LEU:HD23 | 1:73:A:ALA:HA | 2 | 0.21 |
| (1,3649) | 1:129:A:ILE:HG21 | 1:131:A:VAL:H | 1 | 0.21 |
| (1,3649) | 1:129:A:ILE:HG21 | 1:131:A:VAL:H | 16 | 0.21 |
| (1,3617) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HB2 | 8 | 0.21 |
| (1,3617) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HB3 | 8 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 1 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 1 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 1 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 1 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 1 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 1 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 2 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 2 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 2 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 2 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 2 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 2 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 9 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 9 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 9 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 9 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 9 | 0.21 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 9 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 6 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 6 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 6 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 6 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 6 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 6 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 15 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 15 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 15 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 15 | 0.21 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 15 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 15 | 0.21 |
| (1,3516) | 1:58:A:THR:HA | 1:59:A:LEU:HG | 5 | 0.21 |
| (1,3497) | 1:90:A:PHE:HA | 1:92:A:SER:HB2 | 14 | 0.21 |
| (1,3497) | 1:90:A:PHE:HA | 1:92:A:SER:HB3 | 14 | 0.21 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 9 | 0.21 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 9 | 0.21 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 9 | 0.21 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 9 | 0.21 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 9 | 0.21 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 9 | 0.21 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB2 | 16 | 0.21 |
| (1,3490) | 1:17:A:LEU:HD12 | 1:20:A:ARG:HB3 | 16 | 0.21 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB2 | 14 | 0.21 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB3 | 14 | 0.21 |
| (1,3400) | 1:140:A:ILE:HD13 | 1:37:A:THR:HB | 3 | 0.21 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 3 | 0.21 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 5 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HG2 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HG3 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HG2 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HG3 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HG2 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HG3 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG21 | 1:41:A:GLN:HG2 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG21 | 1:41:A:GLN:HG3 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HG2 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HG3 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG23 | 1:41:A:GLN:HG2 | 7 | 0.21 |
| (1,3394) | 1:48:A:VAL:HG23 | 1:41:A:GLN:HG3 | 7 | 0.21 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD11 | 5 | 0.21 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD12 | 5 | 0.21 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD13 | 5 | 0.21 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD21 | 5 | 0.21 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD22 | 5 | 0.21 |
| (1,3320) | 1:99:A:VAL:HG23 | 1:100:A:LEU:HD23 | 5 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 16 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 16 | 0.21 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 16 | 0.21 |
| (1,3255) | 1:124:A:ALA:HB2 | 1:96:A:ASN:HB2 | 9 | 0.21 |
| (1,3255) | 1:124:A:ALA:HB2 | 1:96:A:ASN:HB3 | 9 | 0.21 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA2 | 3 | 0.21 |
| (1,3238) | 1:129:A:ILE:HD11 | 1:128:A:GLY:HA3 | 3 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD2 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD3 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD2 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD3 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD2 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD3 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD2 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD3 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD2 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD3 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD2 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD3 | 7 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD2 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD3 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD2 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD3 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD2 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD3 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD2 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD3 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD2 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD3 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD2 | 18 | 0.21 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD3 | 18 | 0.21 |
| (1,3185) | 1:20:A:ARG:HD2 | 1:191:A:PRO:HA | 7 | 0.21 |
| (1,3185) | 1:20:A:ARG:HD3 | 1:191:A:PRO:HA | 7 | 0.21 |
| (1,3136) | 1:163:A:SER:HB2 | 1:175:A:PRO:HD2 | 3 | 0.21 |
| (1,3136) | 1:163:A:SER:HB2 | 1:175:A:PRO:HD3 | 3 | 0.21 |
| (1,3136) | 1:163:A:SER:HB3 | 1:175:A:PRO:HD2 | 3 | 0.21 |
| (1,3136) | 1:163:A:SER:HB3 | 1:175:A:PRO:HD3 | 3 | 0.21 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG2 | 13 | 0.21 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG3 | 13 | 0.21 |
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG2 | 13 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG3 | 13 | 0.21 |
| (1,3095) | 1:146:A:PHE:HB2 | 1:150:A:SER:HA | 3 | 0.21 |
| (1,3095) | 1:146:A:PHE:HB3 | 1:150:A:SER:HA | 3 | 0.21 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG21 | 18 | 0.21 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG22 | 18 | 0.21 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG23 | 18 | 0.21 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG21 | 18 | 0.21 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG22 | 18 | 0.21 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG23 | 18 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB2 | 1 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB3 | 1 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB2 | 1 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB3 | 1 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB2 | 14 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB2 | 1:148:A:SER:HB3 | 14 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB2 | 14 | 0.21 |
| (1,3082) | 1:147:A:LEU:HB3 | 1:148:A:SER:HB3 | 14 | 0.21 |
| (1,2885) | 1:55:A:LEU:HA | 1:123:A:ALA:HB1 | 4 | 0.21 |
| (1,2885) | 1:55:A:LEU:HA | 1:123:A:ALA:HB2 | 4 | 0.21 |
| (1,2885) | 1:55:A:LEU:HA | 1:123:A:ALA:HB3 | 4 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 7 | 0.21 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 7 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 1 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 1 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 12 | 0.21 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 12 | 0.21 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 6 | 0.21 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 6 | 0.21 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 6 | 0.21 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 6 | 0.21 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 6 | 0.21 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 6 | 0.21 |
| (1,2464) | 1:82:A:ASP:HB2 | 1:83:A:THR:HB | 11 | 0.21 |
| (1,2464) | 1:82:A:ASP:HB3 | 1:83:A:THR:HB | 11 | 0.21 |
| (1,2193) | 1:50:A:ARG:HA | 1:55:A:LEU:HD11 | 6 | 0.21 |
| (1,2193) | 1:50:A:ARG:HA | 1:55:A:LEU:HD12 | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2193) | 1:50:A:ARG:HA | 1:55:A:LEU:HD13 | 6 | 0.21 |
| (1,2193) | 1:50:A:ARG:HA | 1:55:A:LEU:HD21 | 6 | 0.21 |
| (1,2193) | 1:50:A:ARG:HA | 1:55:A:LEU:HD22 | 6 | 0.21 |
| (1,2193) | 1:50:A:ARG:HA | 1:55:A:LEU:HD23 | 6 | 0.21 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 18 | 0.21 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 18 | 0.21 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 15 | 0.21 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 15 | 0.21 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 7 | 0.21 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 7 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG21 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG22 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG23 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG21 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG22 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG23 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG21 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG22 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG23 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG21 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG22 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG23 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG21 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG22 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG23 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG21 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG22 | 16 | 0.21 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG23 | 16 | 0.21 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 5 | 0.21 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG11 | 1 | 0.21 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG12 | 1 | 0.21 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG13 | 1 | 0.21 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG21 | 1 | 0.21 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG22 | 1 | 0.21 |
| (1,1146) | 1:70:A:ALA:H | 1:71:A:VAL:HG23 | 1 | 0.21 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 16 | 0.21 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 16 | 0.21 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 16 | 0.21 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 16 | 0.21 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 16 | 0.21 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 16 | 0.21 |
| (1,1123) | 1:132:A:ASP:H | 1:136:A:VAL:HB | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 1 | 0.21 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 1 | 0.21 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 1 | 0.21 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 2 | 0.21 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 2 | 0.21 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 2 | 0.21 |
| (1,1095) | 1:193:A:GLY:H | 1:191:A:PRO:HA | 11 | 0.21 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 6 | 0.21 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 10 | 0.21 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 10 | 0.21 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 10 | 0.21 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 6 | 0.21 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 12 | 0.21 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 12 | 0.21 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 12 | 0.21 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA2 | 8 | 0.21 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA3 | 8 | 0.21 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 2 | 0.21 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 2 | 0.21 |
| (1,1002) | 1:92:A:SER:H | 1:21:A:VAL:HB | 7 | 0.21 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 1 | 0.21 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 1 | 0.21 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 1 | 0.21 |
| (1,893) | 1:153:A:SER:HB2 | 1:158:A:GLN:H | 6 | 0.21 |
| (1,893) | 1:153:A:SER:HB3 | 1:158:A:GLN:H | 6 | 0.21 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 10 | 0.21 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 10 | 0.21 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 9 | 0.21 |
| (1,781) | 1:127:A:LEU:H | 1:129:A:ILE:H | 12 | 0.21 |
| (1,728) | 1:116:A:LEU:H | 1:120:A:VAL:H | 13 | 0.21 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD21 | 15 | 0.21 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD22 | 15 | 0.21 |
| (1,555) | 1:99:A:VAL:H | 1:100:A:LEU:HG | 17 | 0.21 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 5 | 0.21 |
| (1,295) | 1:50:A:ARG:HB2 | 1:57:A:SER:H | 8 | 0.21 |
| (1,295) | 1:50:A:ARG:HB3 | 1:57:A:SER:H | 8 | 0.21 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 12 | 0.21 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 12 | 0.21 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 4 | 0.2 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 4 | 0.2 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 4 | 0.2 |
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB2 | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3849) | 1:51:A:ALA:HB1 | 1:132:A:ASP:HB3 | 20 | 0.2 |
| (1,3844) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 9 | 0.2 |
| (1,3844) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 13 | 0.2 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB1 | 6 | 0.2 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB2 | 6 | 0.2 |
| (1,3811) | 1:70:A:ALA:HB1 | 1:51:A:ALA:HB3 | 6 | 0.2 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG2 | 2 | 0.2 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG3 | 2 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 10 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 10 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 10 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 10 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 10 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 10 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 16 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 16 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 16 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 16 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 16 | 0.2 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 16 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 15 | 0.2 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 15 | 0.2 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 9 | 0.2 |
| (1,3759) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 9 | 0.2 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 2 | 0.2 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 2 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG21 | 8 | 0.2 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG22 | 8 | 0.2 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG23 | 8 | 0.2 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG21 | 16 | 0.2 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG22 | 16 | 0.2 |
| (1,3707) | 1:86:A:TYR:HB3 | 1:43:A:ILE:HG23 | 16 | 0.2 |
| (1,3695) | 1:195:A:SER:HB2 | 1:102:A:ALA:HA | 4 | 0.2 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG21 | 1 | 0.2 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG22 | 1 | 0.2 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG23 | 1 | 0.2 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG21 | 4 | 0.2 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG22 | 4 | 0.2 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG23 | 4 | 0.2 |
| (1,3654) | 1:39:A:VAL:HG12 | 1:38:A:GLY:HA2 | 17 | 0.2 |
| (1,3654) | 1:39:A:VAL:HG12 | 1:38:A:GLY:HA3 | 17 | 0.2 |
| (1,3645) | 1:94:A:LEU:HD11 | 1:40:A:SER:H | 10 | 0.2 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD11 | 9 | 0.2 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD12 | 9 | 0.2 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD13 | 9 | 0.2 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD21 | 9 | 0.2 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD22 | 9 | 0.2 |
| (1,3644) | 1:113:A:LEU:HD21 | 1:17:A:LEU:HD23 | 9 | 0.2 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 2 | 0.2 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 2 | 0.2 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 3 | 0.2 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 3 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 15 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 15 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 15 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 15 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 15 | 0.2 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 15 | 0.2 |
| (1,3515) | 1:31:A:LEU:HD23 | 1:31:A:LEU:HA | 2 | 0.2 |
| (1,3515) | 1:31:A:LEU:HD23 | 1:31:A:LEU:HA | 9 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD11 | 13 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD12 | 13 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD13 | 13 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD21 | 13 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD22 | 13 | 0.2 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD23 | 13 | 0.2 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 18 | 0.2 |
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB2 | 16 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3422) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HB3 | 16 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 6 | 0.2 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 6 | 0.2 |
| (1,3404) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HG2 | 3 | 0.2 |
| (1,3404) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HG3 | 3 | 0.2 |
| (1,3404) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HG2 | 3 | 0.2 |
| (1,3404) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HG3 | 3 | 0.2 |
| (1,3398) | 1:70:A:ALA:H | 1:68:A:ARG:HA | 18 | 0.2 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB1 | 16 | 0.2 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB2 | 16 | 0.2 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB3 | 16 | 0.2 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 8 | 0.2 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 8 | 0.2 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD11 | 6 | 0.2 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD12 | 6 | 0.2 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD13 | 6 | 0.2 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD21 | 6 | 0.2 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD22 | 6 | 0.2 |
| (1,3320) | 1:99:A:VAL:HG22 | 1:100:A:LEU:HD23 | 6 | 0.2 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 9 | 0.2 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 9 | 0.2 |
| (1,3268) | 1:9:A:ALA:HA | 1:113:A:LEU:HG | 8 | 0.2 |
| (1,3256) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 13 | 0.2 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG2 | 19 | 0.2 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG3 | 19 | 0.2 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG2 | 19 | 0.2 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG3 | 19 | 0.2 |
| (1,2975) | 1:131:A:VAL:HG11 | 1:132:A:ASP:HA | 9 | 0.2 |
| (1,2975) | 1:131:A:VAL:HG12 | 1:132:A:ASP:HA | 9 | 0.2 |
| (1,2975) | 1:131:A:VAL:HG13 | 1:132:A:ASP:HA | 9 | 0.2 |
| (1,2975) | 1:131:A:VAL:HG21 | 1:132:A:ASP:HA | 9 | 0.2 |
| (1,2975) | 1:131:A:VAL:HG22 | 1:132:A:ASP:HA | 9 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2975) | 1:131:A:VAL:HG23 | 1:132:A:ASP:HA | 9 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG11 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG12 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG13 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG21 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG22 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG23 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG11 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG12 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG13 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG21 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG22 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG23 | 2 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG11 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG12 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG13 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG21 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG22 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG23 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG11 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG12 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG13 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG21 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG22 | 6 | 0.2 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG23 | 6 | 0.2 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 6 | 0.2 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 6 | 0.2 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 6 | 0.2 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 6 | 0.2 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 6 | 0.2 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 6 | 0.2 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE21 | 20 | 0.2 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE22 | 20 | 0.2 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE21 | 20 | 0.2 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE22 | 20 | 0.2 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE21 | 20 | 0.2 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE22 | 20 | 0.2 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD2 | 14 | 0.2 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD3 | 14 | 0.2 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 6 | 0.2 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 6 | 0.2 |
| (1,2112) | 1:41:A:GLN:HE21 | 1:45:A:SER:HA | 8 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2112) | 1:41:A:GLN:HE22 | 1:45:A:SER:HA | 8 | 0.2 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB2 | 18 | 0.2 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB3 | 18 | 0.2 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD11 | 3 | 0.2 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD12 | 3 | 0.2 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD13 | 3 | 0.2 |
| (1,1065) | 1:50:A:ARG:HB3 | 1:50:A:ARG:HE | 19 | 0.2 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 2 | 0.2 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 2 | 0.2 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 2 | 0.2 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 9 | 0.2 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 13 | 0.2 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 7 | 0.2 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 7 | 0.2 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 7 | 0.2 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 7 | 0.2 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 7 | 0.2 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 7 | 0.2 |
| (1,1028) | 1:71:A:VAL:H | 1:66:A:LEU:HA | 7 | 0.2 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 7 | 0.2 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 7 | 0.2 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 1 | 0.2 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 1 | 0.2 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 9 | 0.2 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 9 | 0.2 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 10 | 0.2 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD2 | 17 | 0.2 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD3 | 17 | 0.2 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD2 | 10 | 0.2 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD3 | 10 | 0.2 |
| (1,893) | 1:153:A:SER:HB2 | 1:158:A:GLN:H | 19 | 0.2 |
| (1,893) | 1:153:A:SER:HB3 | 1:158:A:GLN:H | 19 | 0.2 |
| (1,885) | 1:154:A:ALA:HA | 1:156:A:TYR:H | 10 | 0.2 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB2 | 6 | 0.2 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB3 | 6 | 0.2 |
| (1,869) | 1:144:A:SER:H | 1:147:A:LEU:HD11 | 3 | 0.2 |
| (1,869) | 1:144:A:SER:H | 1:147:A:LEU:HD12 | 3 | 0.2 |
| (1,869) | 1:144:A:SER:H | 1:147:A:LEU:HD13 | 3 | 0.2 |
| (1,869) | 1:144:A:SER:H | 1:147:A:LEU:HD21 | 3 | 0.2 |
| (1,869) | 1:144:A:SER:H | 1:147:A:LEU:HD22 | 3 | 0.2 |
| (1,869) | 1:144:A:SER:H | 1:147:A:LEU:HD23 | 3 | 0.2 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 19 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 19 | 0.2 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 9 | 0.2 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 9 | 0.2 |
| (1,810) | 1:71:A:VAL:HG11 | 1:134:A:GLY:H | 17 | 0.2 |
| (1,810) | 1:71:A:VAL:HG12 | 1:134:A:GLY:H | 17 | 0.2 |
| (1,810) | 1:71:A:VAL:HG13 | 1:134:A:GLY:H | 17 | 0.2 |
| (1,810) | 1:71:A:VAL:HG21 | 1:134:A:GLY:H | 17 | 0.2 |
| (1,810) | 1:71:A:VAL:HG22 | 1:134:A:GLY:H | 17 | 0.2 |
| (1,810) | 1:71:A:VAL:HG23 | 1:134:A:GLY:H | 17 | 0.2 |
| (1,365) | 1:68:A:ARG:HG2 | 1:69:A:PHE:H | 16 | 0.2 |
| (1,365) | 1:68:A:ARG:HG3 | 1:69:A:PHE:H | 16 | 0.2 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 16 | 0.2 |
| (1,11) | 1:4:A:GLN:H | 1:8:A:GLY:H | 8 | 0.2 |
| (1,11) | 1:4:A:GLN:H | 1:8:A:GLY:H | 17 | 0.2 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 15 | 0.19 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 15 | 0.19 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 6 | 0.19 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 6 | 0.19 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 6 | 0.19 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 6 | 0.19 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 6 | 0.19 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 6 | 0.19 |
| (1,3796) | 1:124:A:ALA:HB3 | 1:120:A:VAL:HA | 16 | 0.19 |
| (1,3796) | 1:124:A:ALA:HB2 | 1:120:A:VAL:HA | 19 | 0.19 |
| (1,3781) | 1:71:A:VAL:HG12 | 1:68:A:ARG:HG2 | 12 | 0.19 |
| (1,3781) | 1:71:A:VAL:HG12 | 1:68:A:ARG:HG3 | 12 | 0.19 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG2 | 14 | 0.19 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG3 | 14 | 0.19 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 3 | 0.19 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 3 | 0.19 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 3 | 0.19 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 3 | 0.19 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 3 | 0.19 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 3 | 0.19 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB2 | 16 | 0.19 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB3 | 16 | 0.19 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG21 | 1 | 0.19 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG22 | 1 | 0.19 |
| (1,3753) | 1:15:A:ALA:HB2 | 1:18:A:ILE:HG23 | 1 | 0.19 |
| (1,3736) | 1:191:A:PRO:HB2 | 1:190:A:ALA:HB1 | 2 | 0.19 |
| (1,3736) | 1:191:A:PRO:HB2 | 1:190:A:ALA:HB2 | 2 | 0.19 |
| (1,3736) | 1:191:A:PRO:HB2 | 1:190:A:ALA:HB3 | 2 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3736) | 1:191:A:PRO:HB3 | 1:190:A:ALA:HB1 | 2 | 0.19 |
| (1,3736) | 1:191:A:PRO:HB3 | 1:190:A:ALA:HB2 | 2 | 0.19 |
| (1,3736) | 1:191:A:PRO:HB3 | 1:190:A:ALA:HB3 | 2 | 0.19 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG21 | 15 | 0.19 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG22 | 15 | 0.19 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG23 | 15 | 0.19 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 12 | 0.19 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 11 | 0.19 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 11 | 0.19 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG21 | 17 | 0.19 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG22 | 17 | 0.19 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG23 | 17 | 0.19 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD11 | 6 | 0.19 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD12 | 6 | 0.19 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD13 | 6 | 0.19 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD21 | 6 | 0.19 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD22 | 6 | 0.19 |
| (1,3644) | 1:113:A:LEU:HD12 | 1:17:A:LEU:HD23 | 6 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 4 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 4 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 4 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 4 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 4 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 4 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 11 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 11 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 11 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 11 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 11 | 0.19 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 11 | 0.19 |
| (1,3583) | 1:74:A:VAL:HG22 | 1:44:A:ALA:HA | 19 | 0.19 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 1 | 0.19 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 1 | 0.19 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 1 | 0.19 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 1 | 0.19 |
| (1,3517) | 1:140:A:ILE:HG22 | 1:30:A:THR:HG21 | 14 | 0.19 |
| (1,3517) | 1:140:A:ILE:HG22 | 1:30:A:THR:HG22 | 14 | 0.19 |
| (1,3517) | 1:140:A:ILE:HG22 | 1:30:A:THR:HG23 | 14 | 0.19 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB1 | 10 | 0.19 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB2 | 10 | 0.19 |
| (1,3500) | 1:129:A:ILE:HG12 | 1:124:A:ALA:HB3 | 10 | 0.19 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD11 | 5 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD12 | 5 | 0.19 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD13 | 5 | 0.19 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD21 | 5 | 0.19 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD22 | 5 | 0.19 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD23 | 5 | 0.19 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD11 | 17 | 0.19 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD12 | 17 | 0.19 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD13 | 17 | 0.19 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD21 | 17 | 0.19 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD22 | 17 | 0.19 |
| (1,3479) | 1:10:A:THR:HA | 1:117:A:LEU:HD23 | 17 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB2 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG11 | 1:195:A:SER:HB3 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB2 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG12 | 1:195:A:SER:HB3 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB2 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG13 | 1:195:A:SER:HB3 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB2 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG21 | 1:195:A:SER:HB3 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB2 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG22 | 1:195:A:SER:HB3 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB2 | 20 | 0.19 |
| (1,3413) | 1:99:A:VAL:HG23 | 1:195:A:SER:HB3 | 20 | 0.19 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 4 | 0.19 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB1 | 5 | 0.19 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB2 | 5 | 0.19 |
| (1,3378) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB3 | 5 | 0.19 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB1 | 7 | 0.19 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB2 | 7 | 0.19 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:56:A:ALA:HB3 | 7 | 0.19 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD11 | 17 | 0.19 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD12 | 17 | 0.19 |
| (1,3344) | 1:93:A:ALA:HB2 | 1:105:A:ILE:HD13 | 17 | 0.19 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD11 | 17 | 0.19 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD12 | 17 | 0.19 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD13 | 17 | 0.19 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD21 | 17 | 0.19 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD22 | 17 | 0.19 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD23 | 17 | 0.19 |
| (1,3251) | 1:71:A:VAL:HB | 1:51:A:ALA:HB1 | 14 | 0.19 |
| (1,3251) | 1:71:A:VAL:HB | 1:51:A:ALA:HB2 | 14 | 0.19 |
| (1,3251) | 1:71:A:VAL:HB | 1:51:A:ALA:HB3 | 14 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD2 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD11 | 1:191:A:PRO:HD3 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD2 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD12 | 1:191:A:PRO:HD3 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD2 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD13 | 1:191:A:PRO:HD3 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD2 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD21 | 1:191:A:PRO:HD3 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD2 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD22 | 1:191:A:PRO:HD3 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD2 | 9 | 0.19 |
| (1,3187) | 1:186:A:LEU:HD23 | 1:191:A:PRO:HD3 | 9 | 0.19 |
| (1,3171) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HA | 6 | 0.19 |
| (1,3171) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HA | 6 | 0.19 |
| (1,3169) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HA | 6 | 0.19 |
| (1,3169) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HA | 6 | 0.19 |
| (1,3136) | 1:163:A:SER:HB2 | 1:175:A:PRO:HD2 | 4 | 0.19 |
| (1,3136) | 1:163:A:SER:HB2 | 1:175:A:PRO:HD3 | 4 | 0.19 |
| (1,3136) | 1:163:A:SER:HB3 | 1:175:A:PRO:HD2 | 4 | 0.19 |
| (1,3136) | 1:163:A:SER:HB3 | 1:175:A:PRO:HD3 | 4 | 0.19 |
| (1,3134) | 1:167:A:ALA:HB1 | 1:175:A:PRO:HG2 | 18 | 0.19 |
| (1,3134) | 1:167:A:ALA:HB1 | 1:175:A:PRO:HG3 | 18 | 0.19 |
| (1,3134) | 1:167:A:ALA:HB2 | 1:175:A:PRO:HG2 | 18 | 0.19 |
| (1,3134) | 1:167:A:ALA:HB2 | 1:175:A:PRO:HG3 | 18 | 0.19 |
| (1,3134) | 1:167:A:ALA:HB3 | 1:175:A:PRO:HG2 | 18 | 0.19 |
| (1,3134) | 1:167:A:ALA:HB3 | 1:175:A:PRO:HG3 | 18 | 0.19 |
| (1,3003) | 1:131:A:VAL:HG11 | 1:136:A:VAL:HB | 11 | 0.19 |
| (1,3003) | 1:131:A:VAL:HG12 | 1:136:A:VAL:HB | 11 | 0.19 |
| (1,3003) | 1:131:A:VAL:HG13 | 1:136:A:VAL:HB | 11 | 0.19 |
| (1,3003) | 1:131:A:VAL:HG21 | 1:136:A:VAL:HB | 11 | 0.19 |
| (1,3003) | 1:131:A:VAL:HG22 | 1:136:A:VAL:HB | 11 | 0.19 |
| (1,3003) | 1:131:A:VAL:HG23 | 1:136:A:VAL:HB | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG11 | 1:134:A:GLY:HA2 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG11 | 1:134:A:GLY:HA3 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG12 | 1:134:A:GLY:HA2 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG12 | 1:134:A:GLY:HA3 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG13 | 1:134:A:GLY:HA2 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG13 | 1:134:A:GLY:HA3 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG21 | 1:134:A:GLY:HA2 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG21 | 1:134:A:GLY:HA3 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG22 | 1:134:A:GLY:HA2 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG22 | 1:134:A:GLY:HA3 | 11 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2980) | 1:131:A:VAL:HG23 | 1:134:A:GLY:HA2 | 11 | 0.19 |
| (1,2980) | 1:131:A:VAL:HG23 | 1:134:A:GLY:HA3 | 11 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 10 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 17 | 0.19 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 17 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG11 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG12 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG13 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG21 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG22 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG23 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG11 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG12 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG13 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG21 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG22 | 14 | 0.19 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG23 | 14 | 0.19 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 3 | 0.19 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 3 | 0.19 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 3 | 0.19 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 3 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD11 | 3 | 0.19 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD12 | 3 | 0.19 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD13 | 3 | 0.19 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD21 | 3 | 0.19 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD22 | 3 | 0.19 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD23 | 3 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 5 | 0.19 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 5 | 0.19 |
| (1,2600) | 1:93:A:ALA:HB1 | 1:96:A:ASN:HB2 | 3 | 0.19 |
| (1,2600) | 1:93:A:ALA:HB1 | 1:96:A:ASN:HB3 | 3 | 0.19 |
| (1,2600) | 1:93:A:ALA:HB2 | 1:96:A:ASN:HB2 | 3 | 0.19 |
| (1,2600) | 1:93:A:ALA:HB2 | 1:96:A:ASN:HB3 | 3 | 0.19 |
| (1,2600) | 1:93:A:ALA:HB3 | 1:96:A:ASN:HB2 | 3 | 0.19 |
| (1,2600) | 1:93:A:ALA:HB3 | 1:96:A:ASN:HB3 | 3 | 0.19 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 15 | 0.19 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 15 | 0.19 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 15 | 0.19 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 15 | 0.19 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 15 | 0.19 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 15 | 0.19 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG2 | 6 | 0.19 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG3 | 6 | 0.19 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD2 | 5 | 0.19 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD3 | 5 | 0.19 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 1 | 0.19 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 1 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 1 | 0.19 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 1 | 0.19 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 1 | 0.19 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 1 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HG11 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HG12 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HG13 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HG21 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HG22 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HG23 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HG11 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HG12 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HG13 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HG21 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HG22 | 7 | 0.19 |
| (1,2245) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HG23 | 7 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG11 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG12 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG13 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG21 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG22 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG23 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG11 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG12 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG13 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG21 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG22 | 17 | 0.19 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG23 | 17 | 0.19 |
| (1,2241) | 1:58:A:THR:HG21 | 1:61:A:VAL:HB | 19 | 0.19 |
| (1,2241) | 1:58:A:THR:HG22 | 1:61:A:VAL:HB | 19 | 0.19 |
| (1,2241) | 1:58:A:THR:HG23 | 1:61:A:VAL:HB | 19 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 4 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 4 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 4 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 6 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 6 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 6 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 7 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 7 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 7 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 8 | 0.19 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 8 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 8 | 0.19 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 20 | 0.19 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 20 | 0.19 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB2 | 10 | 0.19 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB3 | 10 | 0.19 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 2 | 0.19 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 2 | 0.19 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 2 | 0.19 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 2 | 0.19 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 2 | 0.19 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 2 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 10 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 10 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 10 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 11 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 11 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 11 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 18 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 18 | 0.19 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 18 | 0.19 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 5 | 0.19 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 5 | 0.19 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 5 | 0.19 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 16 | 0.19 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 20 | 0.19 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 8 | 0.19 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 8 | 0.19 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 8 | 0.19 |
| (1,1041) | 1:29:A:SER:H | 1:30:A:THR:HB | 6 | 0.19 |
| (1,1039) | 1:90:A:PHE:H | 1:18:A:ILE:HB | 11 | 0.19 |
| (1,1039) | 1:90:A:PHE:H | 1:18:A:ILE:HB | 17 | 0.19 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 20 | 0.19 |
| (1,1023) | 1:164:A:THR:HA | 1:166:A:GLY:H | 18 | 0.19 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 6 | 0.19 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 10 | 0.19 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 10 | 0.19 |
| (1,954) | 1:72:A:GLN:H | 1:68:A:ARG:HA | 9 | 0.19 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA2 | 5 | 0.19 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA3 | 5 | 0.19 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 11 | 0.19 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB2 | 13 | 0.19 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB3 | 13 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 20 | 0.19 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 20 | 0.19 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 14 | 0.19 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 14 | 0.19 |
| (1,783) | 1:50:A:ARG:HD2 | 1:129:A:ILE:H | 19 | 0.19 |
| (1,783) | 1:50:A:ARG:HD3 | 1:129:A:ILE:H | 19 | 0.19 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA2 | 9 | 0.19 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA3 | 9 | 0.19 |
| (1,365) | 1:68:A:ARG:HG2 | 1:69:A:PHE:H | 1 | 0.19 |
| (1,365) | 1:68:A:ARG:HG3 | 1:69:A:PHE:H | 1 | 0.19 |
| (1,352) | 1:66:A:LEU:HG | 1:67:A:ALA:H | 11 | 0.19 |
| (1,276) | 1:50:A:ARG:HB2 | 1:54:A:SER:H | 4 | 0.19 |
| (1,276) | 1:50:A:ARG:HB3 | 1:54:A:SER:H | 4 | 0.19 |
| (1,142) | 1:27:A:ASN:HD21 | 1:32:A:ARG:HE | 15 | 0.19 |
| (1,142) | 1:27:A:ASN:HD22 | 1:32:A:ARG:HE | 15 | 0.19 |
| (1,3913) | 1:99:A:VAL:HG11 | 1:95:A:PHE:HD1 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG11 | 1:95:A:PHE:HD2 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG12 | 1:95:A:PHE:HD1 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG12 | 1:95:A:PHE:HD2 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG13 | 1:95:A:PHE:HD1 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG13 | 1:95:A:PHE:HD2 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG21 | 1:95:A:PHE:HD1 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG21 | 1:95:A:PHE:HD2 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG22 | 1:95:A:PHE:HD1 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG22 | 1:95:A:PHE:HD2 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG23 | 1:95:A:PHE:HD1 | 13 | 0.18 |
| (1,3913) | 1:99:A:VAL:HG23 | 1:95:A:PHE:HD2 | 13 | 0.18 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD1 | 1 | 0.18 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD2 | 1 | 0.18 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD1 | 1 | 0.18 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD2 | 1 | 0.18 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD1 | 1 | 0.18 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD2 | 1 | 0.18 |
| (1,3790) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HA | 9 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 10 | 0.18 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 10 | 0.18 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG21 | 19 | 0.18 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG22 | 19 | 0.18 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG23 | 19 | 0.18 |
| (1,3712) | 1:84:A:SER:HB2 | 1:85:A:ALA:HA | 10 | 0.18 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 20 | 0.18 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 20 | 0.18 |
| (1,3683) | 1:56:A:ALA:HB2 | 1:50:A:ARG:HA | 20 | 0.18 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 6 | 0.18 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 6 | 0.18 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 6 | 0.18 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 6 | 0.18 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 6 | 0.18 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 6 | 0.18 |
| (1,3587) | 1:131:A:VAL:HB | 1:51:A:ALA:HB1 | 7 | 0.18 |
| (1,3587) | 1:131:A:VAL:HB | 1:51:A:ALA:HB2 | 7 | 0.18 |
| (1,3587) | 1:131:A:VAL:HB | 1:51:A:ALA:HB3 | 7 | 0.18 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB2 | 10 | 0.18 |
| (1,3554) | 1:13:A:ALA:HB2 | 1:104:A:ASN:HB3 | 10 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 2 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 2 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 17 | 0.18 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 17 | 0.18 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 19 | 0.18 |
| (1,3455) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 19 | 0.18 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB1 | 12 | 0.18 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB2 | 12 | 0.18 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB3 | 12 | 0.18 |
| (1,3374) | 1:93:A:ALA:HB3 | 1:90:A:PHE:HA | 8 | 0.18 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB1 | 15 | 0.18 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB2 | 15 | 0.18 |
| (1,3372) | 1:53:A:GLN:HB2 | 1:52:A:ALA:HB3 | 15 | 0.18 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB1 | 16 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB2 | 16 | 0.18 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB3 | 16 | 0.18 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 1 | 0.18 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 1 | 0.18 |
| (1,3322) | 1:108:A:LEU:HD22 | 1:107:A:THR:HB | 18 | 0.18 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 12 | 0.18 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 12 | 0.18 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 12 | 0.18 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 12 | 0.18 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 2 | 0.18 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 2 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB2 | 16 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB3 | 16 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB2 | 16 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB3 | 16 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB2 | 16 | 0.18 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB3 | 16 | 0.18 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG21 | 1 | 0.18 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG22 | 1 | 0.18 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG23 | 1 | 0.18 |
| (1,3133) | 1:169:A:TYR:HB2 | 1:175:A:PRO:HD2 | 4 | 0.18 |
| (1,3133) | 1:169:A:TYR:HB2 | 1:175:A:PRO:HD3 | 4 | 0.18 |
| (1,3133) | 1:169:A:TYR:HB3 | 1:175:A:PRO:HD2 | 4 | 0.18 |
| (1,3133) | 1:169:A:TYR:HB3 | 1:175:A:PRO:HD3 | 4 | 0.18 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB2 | 8 | 0.18 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB3 | 8 | 0.18 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA2 | 2 | 0.18 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA3 | 2 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG11 | 1:134:A:GLY:HA2 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG11 | 1:134:A:GLY:HA3 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG12 | 1:134:A:GLY:HA2 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG12 | 1:134:A:GLY:HA3 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG13 | 1:134:A:GLY:HA2 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG13 | 1:134:A:GLY:HA3 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG21 | 1:134:A:GLY:HA2 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG21 | 1:134:A:GLY:HA3 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG22 | 1:134:A:GLY:HA2 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG22 | 1:134:A:GLY:HA3 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG23 | 1:134:A:GLY:HA2 | 9 | 0.18 |
| (1,2980) | 1:131:A:VAL:HG23 | 1:134:A:GLY:HA3 | 9 | 0.18 |
| (1,2970) | 1:37:A:THR:HA | 1:131:A:VAL:HB | 11 | 0.18 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB2 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB3 | 9 | 0.18 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB2 | 9 | 0.18 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB3 | 9 | 0.18 |
| (1,2846) | 1:117:A:LEU:HG | 1:118:A:ASN:HD21 | 13 | 0.18 |
| (1,2846) | 1:117:A:LEU:HG | 1:118:A:ASN:HD22 | 13 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD11 | 10 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD12 | 10 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD13 | 10 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD21 | 10 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD22 | 10 | 0.18 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD23 | 10 | 0.18 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 8 | 0.18 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 8 | 0.18 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 8 | 0.18 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 8 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 6 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 11 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 11 | 0.18 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 11 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG2 | 1:94:A:LEU:HD11 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG2 | 1:94:A:LEU:HD12 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG2 | 1:94:A:LEU:HD13 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG2 | 1:94:A:LEU:HD21 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG2 | 1:94:A:LEU:HD22 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG2 | 1:94:A:LEU:HD23 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG3 | 1:94:A:LEU:HD11 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG3 | 1:94:A:LEU:HD12 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG3 | 1:94:A:LEU:HD13 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG3 | 1:94:A:LEU:HD21 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG3 | 1:94:A:LEU:HD22 | 3 | 0.18 |
| (1,2583) | 1:36:A:ARG:HG3 | 1:94:A:LEU:HD23 | 3 | 0.18 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 16 | 0.18 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 16 | 0.18 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 16 | 0.18 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 16 | 0.18 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 16 | 0.18 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 16 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 15 | 0.18 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 15 | 0.18 |
| (1,2280) | 1:62:A:ASP:HA | 1:66:A:LEU:HG | 4 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG11 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG12 | 15 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG13 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG21 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG22 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG23 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG11 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG12 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG13 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG21 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG22 | 15 | 0.18 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG23 | 15 | 0.18 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 3 | 0.18 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 3 | 0.18 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 3 | 0.18 |
| (1,2177) | 1:50:A:ARG:HD2 | 1:54:A:SER:HB2 | 3 | 0.18 |
| (1,2177) | 1:50:A:ARG:HD2 | 1:54:A:SER:HB3 | 3 | 0.18 |
| (1,2177) | 1:50:A:ARG:HD3 | 1:54:A:SER:HB2 | 3 | 0.18 |
| (1,2177) | 1:50:A:ARG:HD3 | 1:54:A:SER:HB3 | 3 | 0.18 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 15 | 0.18 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 15 | 0.18 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 1 | 0.18 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 1 | 0.18 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 4 | 0.18 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 4 | 0.18 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 20 | 0.18 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 20 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG21 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG22 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG23 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG21 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG22 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG23 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG21 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG22 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG23 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG21 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG22 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG23 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG21 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG22 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG23 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG21 | 17 | 0.18 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG22 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG23 | 17 | 0.18 |
| (1,1803) | 1:177:A:THR:H | 1:175:A:PRO:HA | 6 | 0.18 |
| (1,1736) | 1:176:A:SER:HA | 1:177:A:THR:H | 2 | 0.18 |
| (1,1641) | 1:127:A:LEU:H | 1:127:A:LEU:HG | 14 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 2 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 2 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 2 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 2 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 2 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 2 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 12 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 12 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 12 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 12 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 12 | 0.18 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 12 | 0.18 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB1 | 17 | 0.18 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB2 | 17 | 0.18 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB3 | 17 | 0.18 |
| (1,1113) | 1:65:A:ASN:HD21 | 1:47:A:VAL:HB | 16 | 0.18 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 6 | 0.18 |
| (1,1095) | 1:193:A:GLY:H | 1:191:A:PRO:HA | 4 | 0.18 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 1 | 0.18 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 2 | 0.18 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA2 | 15 | 0.18 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA3 | 15 | 0.18 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 17 | 0.18 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 17 | 0.18 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 17 | 0.18 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD11 | 16 | 0.18 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD12 | 16 | 0.18 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD13 | 16 | 0.18 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD21 | 16 | 0.18 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD22 | 16 | 0.18 |
| (1,1054) | 1:56:A:ALA:H | 1:55:A:LEU:HD23 | 16 | 0.18 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 12 | 0.18 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 12 | 0.18 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 12 | 0.18 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 12 | 0.18 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 12 | 0.18 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 12 | 0.18 |
| (1,1028) | 1:71:A:VAL:H | 1:66:A:LEU:HA | 19 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,999) | 1:134:A:GLY:HA2 | 1:132:A:ASP:H | 1 | 0.18 |
| (1,999) | 1:134:A:GLY:HA3 | 1:132:A:ASP:H | 1 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 13 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 13 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 13 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 13 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 13 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 13 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 14 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 14 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 14 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 14 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 14 | 0.18 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 14 | 0.18 |
| (1,917) | 1:161:A:ALA:H | 1:177:A:THR:HB | 6 | 0.18 |
| (1,885) | 1:154:A:ALA:HA | 1:156:A:TYR:H | 18 | 0.18 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB2 | 14 | 0.18 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB3 | 14 | 0.18 |
| (1,792) | 1:38:A:GLY:HA2 | 1:131:A:VAL:H | 15 | 0.18 |
| (1,792) | 1:38:A:GLY:HA3 | 1:131:A:VAL:H | 15 | 0.18 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 8 | 0.18 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA2 | 6 | 0.18 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA3 | 6 | 0.18 |
| (1,589) | 1:101:A:ASN:H | 1:104:A:ASN:H | 4 | 0.18 |
| (1,362) | 1:66:A:LEU:HG | 1:68:A:ARG:H | 19 | 0.18 |
| (1,352) | 1:66:A:LEU:HG | 1:67:A:ALA:H | 10 | 0.18 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB2 | 20 | 0.18 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB3 | 20 | 0.18 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 7 | 0.18 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 8 | 0.18 |
| (1,123) | 1:31:A:LEU:H | 1:31:A:LEU:HG | 2 | 0.18 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 14 | 0.17 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 14 | 0.17 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 6 | 0.17 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 6 | 0.17 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 15 | 0.17 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 15 | 0.17 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 15 | 0.17 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 15 | 0.17 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 15 | 0.17 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 15 | 0.17 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB1 | 15 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB2 | 15 | 0.17 |
| (1,3864) | 1:11:A:GLY:H | 1:93:A:ALA:HB3 | 15 | 0.17 |
| (1,3844) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 14 | 0.17 |
| (1,3836) | 1:71:A:VAL:HG11 | 1:66:A:LEU:HA | 19 | 0.17 |
| (1,3836) | 1:71:A:VAL:HG12 | 1:66:A:LEU:HA | 19 | 0.17 |
| (1,3836) | 1:71:A:VAL:HG13 | 1:66:A:LEU:HA | 19 | 0.17 |
| (1,3836) | 1:71:A:VAL:HG21 | 1:66:A:LEU:HA | 19 | 0.17 |
| (1,3836) | 1:71:A:VAL:HG22 | 1:66:A:LEU:HA | 19 | 0.17 |
| (1,3836) | 1:71:A:VAL:HG23 | 1:66:A:LEU:HA | 19 | 0.17 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG2 | 18 | 0.17 |
| (1,3781) | 1:21:A:VAL:HG21 | 1:20:A:ARG:HG3 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 18 | 0.17 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 18 | 0.17 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB2 | 1 | 0.17 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB3 | 1 | 0.17 |
| (1,3735) | 1:48:A:VAL:HG22 | 1:46:A:SER:H | 1 | 0.17 |
| (1,3695) | 1:150:A:SER:HB2 | 1:147:A:LEU:HA | 15 | 0.17 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG21 | 3 | 0.17 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG22 | 3 | 0.17 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG23 | 3 | 0.17 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 18 | 0.17 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 18 | 0.17 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE21 | 13 | 0.17 |
| (1,3606) | 1:35:A:LEU:HD22 | 1:88:A:GLN:HE22 | 13 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 8 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 8 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 8 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 8 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 8 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 8 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 13 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 13 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 13 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 13 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 13 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 13 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 14 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 14 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 14 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 14 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 14 | 0.17 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 14 | 0.17 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD11 | 2 | 0.17 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD12 | 2 | 0.17 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD13 | 2 | 0.17 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD21 | 2 | 0.17 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD22 | 2 | 0.17 |
| (1,3579) | 1:43:A:ILE:HD13 | 1:77:A:LEU:HD23 | 2 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 12 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 12 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 12 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 12 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 12 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 12 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB1 | 16 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB2 | 16 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD1 | 1:44:A:ALA:HB3 | 16 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB1 | 16 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB2 | 16 | 0.17 |
| (1,3574) | 1:86:A:TYR:HD2 | 1:44:A:ALA:HB3 | 16 | 0.17 |
| (1,3545) | 1:55:A:LEU:HD21 | 1:49:A:GLN:HB2 | 4 | 0.17 |
| (1,3545) | 1:55:A:LEU:HD21 | 1:49:A:GLN:HB3 | 4 | 0.17 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG2 | 14 | 0.17 |
| (1,3520) | 1:129:A:ILE:HG12 | 1:50:A:ARG:HG3 | 14 | 0.17 |
| (1,3515) | 1:31:A:LEU:HD22 | 1:31:A:LEU:HA | 6 | 0.17 |
| (1,3515) | 1:31:A:LEU:HD23 | 1:31:A:LEU:HA | 16 | 0.17 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB1 | 6 | 0.17 |
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB2 | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3500) | 1:129:A:ILE:HG13 | 1:124:A:ALA:HB3 | 6 | 0.17 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 4 | 0.17 |
| (1,3455) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 4 | 0.17 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB2 | 16 | 0.17 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB3 | 16 | 0.17 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD2 | 12 | 0.17 |
| (1,3421) | 1:193:A:GLY:HA2 | 1:191:A:PRO:HD3 | 12 | 0.17 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD2 | 12 | 0.17 |
| (1,3421) | 1:193:A:GLY:HA3 | 1:191:A:PRO:HD3 | 12 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 17 | 0.17 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 17 | 0.17 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 11 | 0.17 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 13 | 0.17 |
| (1,3387) | 1:125:A:GLN:HA | 1:128:A:GLY:HA2 | 12 | 0.17 |
| (1,3387) | 1:125:A:GLN:HA | 1:128:A:GLY:HA3 | 12 | 0.17 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 17 | 0.17 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 17 | 0.17 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 17 | 0.17 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 17 | 0.17 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB2 | 15 | 0.17 |
| (1,3287) | 1:122:A:SER:HB2 | 1:121:A:SER:HB3 | 15 | 0.17 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB2 | 15 | 0.17 |
| (1,3287) | 1:122:A:SER:HB3 | 1:121:A:SER:HB3 | 15 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG2 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3200) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3200) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG2 | 7 | 0.17 |
| (1,3199) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG3 | 7 | 0.17 |
| (1,3190) | 1:17:A:LEU:HB2 | 1:191:A:PRO:HB2 | 8 | 0.17 |
| (1,3190) | 1:17:A:LEU:HB2 | 1:191:A:PRO:HB3 | 8 | 0.17 |
| (1,3190) | 1:17:A:LEU:HB3 | 1:191:A:PRO:HB2 | 8 | 0.17 |
| (1,3190) | 1:17:A:LEU:HB3 | 1:191:A:PRO:HB3 | 8 | 0.17 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 17 | 0.17 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 17 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 18 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 18 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 18 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 18 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB2 | 18 | 0.17 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB3 | 18 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG21 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG22 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG23 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG21 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG22 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG23 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG21 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG22 | 7 | 0.17 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG23 | 7 | 0.17 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB1 | 4 | 0.17 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB2 | 4 | 0.17 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB3 | 4 | 0.17 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG21 | 15 | 0.17 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG22 | 15 | 0.17 |
| (1,3090) | 1:27:A:ASN:HB2 | 1:149:A:THR:HG23 | 15 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG21 | 15 | 0.17 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG22 | 15 | 0.17 |
| (1,3090) | 1:27:A:ASN:HB3 | 1:149:A:THR:HG23 | 15 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG21 | 9 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG22 | 9 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG23 | 9 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG21 | 9 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG22 | 9 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG23 | 9 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG21 | 20 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG22 | 20 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG23 | 20 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG21 | 20 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG22 | 20 | 0.17 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG23 | 20 | 0.17 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB2 | 2 | 0.17 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB3 | 2 | 0.17 |
| (1,3005) | 1:37:A:THR:HG21 | 1:136:A:VAL:HA | 3 | 0.17 |
| (1,3005) | 1:37:A:THR:HG22 | 1:136:A:VAL:HA | 3 | 0.17 |
| (1,3005) | 1:37:A:THR:HG23 | 1:136:A:VAL:HA | 3 | 0.17 |
| (1,3002) | 1:131:A:VAL:HG11 | 1:136:A:VAL:H | 9 | 0.17 |
| (1,3002) | 1:131:A:VAL:HG12 | 1:136:A:VAL:H | 9 | 0.17 |
| (1,3002) | 1:131:A:VAL:HG13 | 1:136:A:VAL:H | 9 | 0.17 |
| (1,3002) | 1:131:A:VAL:HG21 | 1:136:A:VAL:H | 9 | 0.17 |
| (1,3002) | 1:131:A:VAL:HG22 | 1:136:A:VAL:H | 9 | 0.17 |
| (1,3002) | 1:131:A:VAL:HG23 | 1:136:A:VAL:H | 9 | 0.17 |
| (1,2999) | 1:133:A:SER:HA | 1:136:A:VAL:HG11 | 20 | 0.17 |
| (1,2999) | 1:133:A:SER:HA | 1:136:A:VAL:HG12 | 20 | 0.17 |
| (1,2999) | 1:133:A:SER:HA | 1:136:A:VAL:HG13 | 20 | 0.17 |
| (1,2999) | 1:133:A:SER:HA | 1:136:A:VAL:HG21 | 20 | 0.17 |
| (1,2999) | 1:133:A:SER:HA | 1:136:A:VAL:HG22 | 20 | 0.17 |
| (1,2999) | 1:133:A:SER:HA | 1:136:A:VAL:HG23 | 20 | 0.17 |
| (1,2985) | 1:35:A:LEU:HD11 | 1:135:A:SER:HA | 10 | 0.17 |
| (1,2985) | 1:35:A:LEU:HD12 | 1:135:A:SER:HA | 10 | 0.17 |
| (1,2985) | 1:35:A:LEU:HD13 | 1:135:A:SER:HA | 10 | 0.17 |
| (1,2985) | 1:35:A:LEU:HD21 | 1:135:A:SER:HA | 10 | 0.17 |
| (1,2985) | 1:35:A:LEU:HD22 | 1:135:A:SER:HA | 10 | 0.17 |
| (1,2985) | 1:35:A:LEU:HD23 | 1:135:A:SER:HA | 10 | 0.17 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA2 | 11 | 0.17 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA3 | 11 | 0.17 |
| (1,2961) | 1:38:A:GLY:HA2 | 1:130:A:ASN:HA | 6 | 0.17 |
| (1,2961) | 1:38:A:GLY:HA3 | 1:130:A:ASN:HA | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 3 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 18 | 0.17 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 18 | 0.17 |
| (1,2869) | 1:55:A:LEU:HB2 | 1:120:A:VAL:HA | 1 | 0.17 |
| (1,2869) | 1:55:A:LEU:HB3 | 1:120:A:VAL:HA | 1 | 0.17 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD11 | 20 | 0.17 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD12 | 20 | 0.17 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD13 | 20 | 0.17 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD21 | 20 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD22 | 20 | 0.17 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD23 | 20 | 0.17 |
| (1,2731) | 1:108:A:LEU:HG | 1:109:A:GLY:HA2 | 7 | 0.17 |
| (1,2731) | 1:108:A:LEU:HG | 1:109:A:GLY:HA3 | 7 | 0.17 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 11 | 0.17 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 11 | 0.17 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 11 | 0.17 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 11 | 0.17 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 11 | 0.17 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 11 | 0.17 |
| (1,2609) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HA | 20 | 0.17 |
| (1,2609) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HA | 20 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 11 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 11 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 11 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 11 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 11 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 11 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 14 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 14 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 14 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 14 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 14 | 0.17 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 14 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB2 | 1:78:A:PRO:HG2 | 4 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB2 | 1:78:A:PRO:HG3 | 4 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB3 | 1:78:A:PRO:HG2 | 4 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB3 | 1:78:A:PRO:HG3 | 4 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB2 | 1:78:A:PRO:HG2 | 12 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB2 | 1:78:A:PRO:HG3 | 12 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB3 | 1:78:A:PRO:HG2 | 12 | 0.17 |
| (1,2447) | 1:77:A:LEU:HB3 | 1:78:A:PRO:HG3 | 12 | 0.17 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG2 | 14 | 0.17 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG3 | 14 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 3 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 3 | 0.17 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 3 | 0.17 |
| (1,2287) | 1:66:A:LEU:HD11 | 1:67:A:ALA:HA | 2 | 0.17 |
| (1,2287) | 1:66:A:LEU:HD12 | 1:67:A:ALA:HA | 2 | 0.17 |
| (1,2287) | 1:66:A:LEU:HD13 | 1:67:A:ALA:HA | 2 | 0.17 |
| (1,2287) | 1:66:A:LEU:HD21 | 1:67:A:ALA:HA | 2 | 0.17 |
| (1,2287) | 1:66:A:LEU:HD22 | 1:67:A:ALA:HA | 2 | 0.17 |
| (1,2287) | 1:66:A:LEU:HD23 | 1:67:A:ALA:HA | 2 | 0.17 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 12 | 0.17 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 12 | 0.17 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 12 | 0.17 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 16 | 0.17 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 16 | 0.17 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 16 | 0.17 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB2 | 3 | 0.17 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB3 | 3 | 0.17 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD11 | 6 | 0.17 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD12 | 6 | 0.17 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD13 | 6 | 0.17 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD21 | 6 | 0.17 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD22 | 6 | 0.17 |
| (1,2195) | 1:50:A:ARG:H | 1:55:A:LEU:HD23 | 6 | 0.17 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 5 | 0.17 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 5 | 0.17 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 12 | 0.17 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 12 | 0.17 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 4 | 0.17 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 4 | 0.17 |
| (1,1970) | 1:31:A:LEU:HD11 | 1:32:A:ARG:HE | 11 | 0.17 |
| (1,1970) | 1:31:A:LEU:HD12 | 1:32:A:ARG:HE | 11 | 0.17 |
| (1,1970) | 1:31:A:LEU:HD13 | 1:32:A:ARG:HE | 11 | 0.17 |
| (1,1970) | 1:31:A:LEU:HD21 | 1:32:A:ARG:HE | 11 | 0.17 |
| (1,1970) | 1:31:A:LEU:HD22 | 1:32:A:ARG:HE | 11 | 0.17 |
| (1,1970) | 1:31:A:LEU:HD23 | 1:32:A:ARG:HE | 11 | 0.17 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD11 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD12 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD13 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD21 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD22 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD23 | 9 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD11 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD12 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD13 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD21 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD23 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD11 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD12 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD13 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD21 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD22 | 9 | 0.17 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD23 | 9 | 0.17 |
| (1,1803) | 1:177:A:THR:H | 1:175:A:PRO:HA | 15 | 0.17 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 5 | 0.17 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 4 | 0.17 |
| (1,1401) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 5 | 0.17 |
| (1,1401) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 5 | 0.17 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 10 | 0.17 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 10 | 0.17 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 10 | 0.17 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 10 | 0.17 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 10 | 0.17 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 10 | 0.17 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 17 | 0.17 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 7 | 0.17 |
| (1,1107) | 1:109:A:GLY:H | 1:105:A:ILE:HB | 11 | 0.17 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD11 | 14 | 0.17 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD12 | 14 | 0.17 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD13 | 14 | 0.17 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB2 | 18 | 0.17 |
| (1,1008) | 1:40:A:SER:H | 1:42:A:GLN:HB3 | 18 | 0.17 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD11 | 10 | 0.17 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD12 | 10 | 0.17 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD13 | 10 | 0.17 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD21 | 10 | 0.17 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD22 | 10 | 0.17 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD23 | 10 | 0.17 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 11 | 0.17 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 11 | 0.17 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 11 | 0.17 |
| (1,945) | 1:194:A:GLN:HG2 | 1:196:A:GLY:H | 9 | 0.17 |
| (1,945) | 1:194:A:GLN:HG3 | 1:196:A:GLY:H | 9 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 17 | 0.17 |
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 17 | 0.17 |
| (1,927) | 1:179:A:PRO:HD2 | 1:187:A:GLY:H | 5 | 0.17 |
| (1,927) | 1:179:A:PRO:HD3 | 1:187:A:GLY:H | 5 | 0.17 |
| (1,919) | 1:180:A:SER:H | 1:180:A:SER:HB2 | 17 | 0.17 |
| (1,919) | 1:180:A:SER:H | 1:180:A:SER:HB3 | 17 | 0.17 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG2 | 1 | 0.17 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG3 | 1 | 0.17 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 8 | 0.17 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 8 | 0.17 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 5 | 0.17 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 5 | 0.17 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 17 | 0.17 |
| (1,609) | 1:101:A:ASN:H | 1:105:A:ILE:H | 11 | 0.17 |
| (1,594) | 1:100:A:LEU:HD11 | 1:104:A:ASN:H | 5 | 0.17 |
| (1,594) | 1:100:A:LEU:HD12 | 1:104:A:ASN:H | 5 | 0.17 |
| (1,594) | 1:100:A:LEU:HD13 | 1:104:A:ASN:H | 5 | 0.17 |
| (1,594) | 1:100:A:LEU:HD21 | 1:104:A:ASN:H | 5 | 0.17 |
| (1,594) | 1:100:A:LEU:HD22 | 1:104:A:ASN:H | 5 | 0.17 |
| (1,594) | 1:100:A:LEU:HD23 | 1:104:A:ASN:H | 5 | 0.17 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD21 | 8 | 0.17 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD22 | 8 | 0.17 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 5 | 0.17 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD21 | 5 | 0.17 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD22 | 5 | 0.17 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD21 | 5 | 0.17 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD22 | 5 | 0.17 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 4 | 0.17 |
| (1,313) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 5 | 0.17 |
| (1,313) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 5 | 0.17 |
| (1,312) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 5 | 0.17 |
| (1,312) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 5 | 0.17 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD11 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD12 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD13 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD21 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD22 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD21 | 1:31:A:LEU:HD23 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD11 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD12 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD13 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD21 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD22 | 7 | 0.17 |
| (1,127) | 1:27:A:ASN:HD22 | 1:31:A:LEU:HD23 | 7 | 0.17 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 12 | 0.16 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 12 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD1 | 4 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD2 | 4 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD1 | 4 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD2 | 4 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD1 | 4 | 0.16 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD2 | 4 | 0.16 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE1 | 9 | 0.16 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE2 | 9 | 0.16 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE1 | 9 | 0.16 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE2 | 9 | 0.16 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE1 | 9 | 0.16 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE2 | 9 | 0.16 |
| (1,3876) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 18 | 0.16 |
| (1,3876) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 18 | 0.16 |
| (1,3876) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 18 | 0.16 |
| (1,3876) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 18 | 0.16 |
| (1,3876) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 18 | 0.16 |
| (1,3876) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 18 | 0.16 |
| (1,3785) | 1:158:A:GLN:HB3 | 1:161:A:ALA:HB1 | 7 | 0.16 |
| (1,3785) | 1:158:A:GLN:HB3 | 1:161:A:ALA:HB2 | 7 | 0.16 |
| (1,3785) | 1:158:A:GLN:HB3 | 1:161:A:ALA:HB3 | 7 | 0.16 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG2 | 9 | 0.16 |
| (1,3781) | 1:21:A:VAL:HG22 | 1:20:A:ARG:HG3 | 9 | 0.16 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG11 | 4 | 0.16 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG12 | 4 | 0.16 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG13 | 4 | 0.16 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG21 | 4 | 0.16 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG22 | 4 | 0.16 |
| (1,3764) | 1:111:A:ARG:HD3 | 1:112:A:VAL:HG23 | 4 | 0.16 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB2 | 16 | 0.16 |
| (1,3734) | 1:20:A:ARG:HA | 1:191:A:PRO:HB3 | 16 | 0.16 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 6 | 0.16 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 6 | 0.16 |
| (1,3614) | 1:177:A:THR:HG21 | 1:175:A:PRO:HG2 | 9 | 0.16 |
| (1,3614) | 1:177:A:THR:HG21 | 1:175:A:PRO:HG3 | 9 | 0.16 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE21 | 17 | 0.16 |
| (1,3606) | 1:35:A:LEU:HD21 | 1:88:A:GLN:HE22 | 17 | 0.16 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 18 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 18 | 0.16 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 18 | 0.16 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 18 | 0.16 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 18 | 0.16 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 18 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB1 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB2 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB3 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB1 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB2 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB3 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB1 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB2 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB3 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB1 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB2 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB3 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB1 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB2 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB3 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB1 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB2 | 20 | 0.16 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB3 | 20 | 0.16 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 6 | 0.16 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 6 | 0.16 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 6 | 0.16 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 6 | 0.16 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD11 | 6 | 0.16 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD12 | 6 | 0.16 |
| (1,3493) | 1:23:A:ASN:HB2 | 1:18:A:ILE:HD13 | 6 | 0.16 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD11 | 6 | 0.16 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD12 | 6 | 0.16 |
| (1,3493) | 1:23:A:ASN:HB3 | 1:18:A:ILE:HD13 | 6 | 0.16 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB2 | 3 | 0.16 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB3 | 3 | 0.16 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB2 | 3 | 0.16 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB3 | 3 | 0.16 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 11 | 0.16 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 15 | 0.16 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 15 | 0.16 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 15 | 0.16 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 15 | 0.16 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 15 | 0.16 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 16 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HG2 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG11 | 1:41:A:GLN:HG3 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HG2 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG12 | 1:41:A:GLN:HG3 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HG2 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HG3 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG21 | 1:41:A:GLN:HG2 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG21 | 1:41:A:GLN:HG3 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HG2 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG22 | 1:41:A:GLN:HG3 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG23 | 1:41:A:GLN:HG2 | 14 | 0.16 |
| (1,3394) | 1:48:A:VAL:HG23 | 1:41:A:GLN:HG3 | 14 | 0.16 |
| (1,3285) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 18 | 0.16 |
| (1,3285) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 18 | 0.16 |
| (1,3285) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 18 | 0.16 |
| (1,3285) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 18 | 0.16 |
| (1,3285) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 18 | 0.16 |
| (1,3285) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 18 | 0.16 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 19 | 0.16 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 19 | 0.16 |
| (1,3214) | 1:14:A:SER:HB2 | 1:18:A:ILE:HD11 | 1 | 0.16 |
| (1,3214) | 1:14:A:SER:HB2 | 1:18:A:ILE:HD12 | 1 | 0.16 |
| (1,3214) | 1:14:A:SER:HB2 | 1:18:A:ILE:HD13 | 1 | 0.16 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD2 | 19 | 0.16 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD3 | 19 | 0.16 |
| (1,3173) | 1:177:A:THR:HG21 | 1:190:A:ALA:HA | 16 | 0.16 |
| (1,3173) | 1:177:A:THR:HG22 | 1:190:A:ALA:HA | 16 | 0.16 |
| (1,3173) | 1:177:A:THR:HG23 | 1:190:A:ALA:HA | 16 | 0.16 |
| (1,3160) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HG | 15 | 0.16 |
| (1,3160) | 1:185:A:PRO:HG3 | 1:186:A:LEU:HG | 15 | 0.16 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB2 | 3 | 0.16 |
| (1,3132) | 1:161:A:ALA:HB1 | 1:175:A:PRO:HB3 | 3 | 0.16 |
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB2 | 3 | 0.16 |
| (1,3132) | 1:161:A:ALA:HB2 | 1:175:A:PRO:HB3 | 3 | 0.16 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB2 | 3 | 0.16 |
| (1,3132) | 1:161:A:ALA:HB3 | 1:175:A:PRO:HB3 | 3 | 0.16 |
| (1,3122) | 1:20:A:ARG:HG2 | 1:171:A:GLY:HA2 | 1 | 0.16 |
| (1,3122) | 1:20:A:ARG:HG2 | 1:171:A:GLY:HA3 | 1 | 0.16 |
| (1,3122) | 1:20:A:ARG:HG3 | 1:171:A:GLY:HA2 | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3122) | 1:20:A:ARG:HG3 | 1:171:A:GLY:HA3 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG21 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG22 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG23 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG21 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG22 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG23 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG21 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG22 | 1 | 0.16 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG23 | 1 | 0.16 |
| (1,3114) | 1:163:A:SER:HA | 1:167:A:ALA:HB1 | 12 | 0.16 |
| (1,3114) | 1:163:A:SER:HA | 1:167:A:ALA:HB2 | 12 | 0.16 |
| (1,3114) | 1:163:A:SER:HA | 1:167:A:ALA:HB3 | 12 | 0.16 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB1 | 1 | 0.16 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB2 | 1 | 0.16 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB3 | 1 | 0.16 |
| (1,3021) | 1:28:A:THR:HG21 | 1:139:A:ASP:HA | 2 | 0.16 |
| (1,3021) | 1:28:A:THR:HG22 | 1:139:A:ASP:HA | 2 | 0.16 |
| (1,3021) | 1:28:A:THR:HG23 | 1:139:A:ASP:HA | 2 | 0.16 |
| (1,3005) | 1:37:A:THR:HG21 | 1:136:A:VAL:HA | 11 | 0.16 |
| (1,3005) | 1:37:A:THR:HG22 | 1:136:A:VAL:HA | 11 | 0.16 |
| (1,3005) | 1:37:A:THR:HG23 | 1:136:A:VAL:HA | 11 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 6 | 0.16 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB2 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB3 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB2 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB3 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB2 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB3 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB2 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB3 | 6 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB2 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB3 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB2 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB3 | 6 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB2 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB3 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB2 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB3 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB2 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB3 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB2 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB3 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB2 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB3 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB2 | 18 | 0.16 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB3 | 18 | 0.16 |
| (1,2835) | 1:110:A:SER:HA | 1:117:A:LEU:HA | 8 | 0.16 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 20 | 0.16 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 20 | 0.16 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 20 | 0.16 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 20 | 0.16 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 20 | 0.16 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 20 | 0.16 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 20 | 0.16 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 20 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 12 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 9 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 9 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 12 | 0.16 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 12 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 12 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 2 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 2 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 2 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 2 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 2 | 0.16 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 2 | 0.16 |
| (1,2520) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 18 | 0.16 |
| (1,2520) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 18 | 0.16 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE21 | 13 | 0.16 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE22 | 13 | 0.16 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE21 | 13 | 0.16 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE22 | 13 | 0.16 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE21 | 13 | 0.16 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE22 | 13 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD1 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD2 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD1 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD2 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD1 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD2 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD1 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD2 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD1 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD2 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD1 | 17 | 0.16 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD2 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE1 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE2 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE1 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE2 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE1 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE2 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE1 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE2 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE1 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE2 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE1 | 17 | 0.16 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE2 | 17 | 0.16 |
| (1,2280) | 1:62:A:ASP:HA | 1:66:A:LEU:HG | 13 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD21 | 1 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD22 | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD21 | 1 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD22 | 1 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD21 | 16 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD22 | 16 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD21 | 16 | 0.16 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD22 | 16 | 0.16 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 10 | 0.16 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 10 | 0.16 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 10 | 0.16 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 10 | 0.16 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 14 | 0.16 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 14 | 0.16 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG21 | 9 | 0.16 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG22 | 9 | 0.16 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG23 | 9 | 0.16 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG21 | 9 | 0.16 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG22 | 9 | 0.16 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG23 | 9 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG11 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG12 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG13 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG21 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG22 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG23 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG11 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG12 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG13 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG21 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG22 | 11 | 0.16 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG23 | 11 | 0.16 |
| (1,1868) | 1:18:A:ILE:HB | 1:19:A:SER:HB2 | 11 | 0.16 |
| (1,1868) | 1:18:A:ILE:HB | 1:19:A:SER:HB3 | 11 | 0.16 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 1 | 0.16 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 13 | 0.16 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 8 | 0.16 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 9 | 0.16 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 11 | 0.16 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 14 | 0.16 |
| (1,1403) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 9 | 0.16 |
| (1,1403) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 9 | 0.16 |
| (1,1183) | 1:67:A:ALA:H | 1:66:A:LEU:H | 8 | 0.16 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 2 | 0.16 |
| (1,1138) | 1:76:A:ARG:HB3 | 1:74:A:VAL:H | 13 | 0.16 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG21 | 6 | 0.16 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG22 | 6 | 0.16 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG23 | 6 | 0.16 |
| (1,1130) | 1:186:A:LEU:H | 1:187:A:GLY:HA2 | 8 | 0.16 |
| (1,1130) | 1:186:A:LEU:H | 1:187:A:GLY:HA3 | 8 | 0.16 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 3 | 0.16 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 3 | 0.16 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 3 | 0.16 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 6 | 0.16 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 6 | 0.16 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 6 | 0.16 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA2 | 18 | 0.16 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA3 | 18 | 0.16 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 3 | 0.16 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 3 | 0.16 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 3 | 0.16 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 4 | 0.16 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 4 | 0.16 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 5 | 0.16 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 5 | 0.16 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 5 | 0.16 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 5 | 0.16 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 5 | 0.16 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 5 | 0.16 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA2 | 7 | 0.16 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA3 | 7 | 0.16 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 13 | 0.16 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 13 | 0.16 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 16 | 0.16 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 16 | 0.16 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 16 | 0.16 |
| (1,946) | 1:196:A:GLY:H | 1:197:A:PHE:HA | 3 | 0.16 |
| (1,945) | 1:194:A:GLN:HG2 | 1:196:A:GLY:H | 2 | 0.16 |
| (1,945) | 1:194:A:GLN:HG3 | 1:196:A:GLY:H | 2 | 0.16 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 5 | 0.16 |
| (1,781) | 1:127:A:LEU:H | 1:129:A:ILE:H | 3 | 0.16 |
| (1,781) | 1:127:A:LEU:H | 1:129:A:ILE:H | 11 | 0.16 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA2 | 15 | 0.16 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA3 | 15 | 0.16 |
| (1,455) | 1:83:A:THR:HG21 | 1:84:A:SER:H | 17 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,455) | 1:83:A:THR:HG22 | 1:84:A:SER:H | 17 | 0.16 |
| (1,455) | 1:83:A:THR:HG23 | 1:84:A:SER:H | 17 | 0.16 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 1 | 0.16 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 13 | 0.16 |
| (1,332) | 1:61:A:VAL:HA | 1:64:A:ASN:H | 12 | 0.16 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 8 | 0.16 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 9 | 0.16 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 11 | 0.16 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 14 | 0.16 |
| (1,315) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 9 | 0.16 |
| (1,315) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 9 | 0.16 |
| (1,268) | 1:50:A:ARG:HG2 | 1:53:A:GLN:H | 8 | 0.16 |
| (1,268) | 1:50:A:ARG:HG3 | 1:53:A:GLN:H | 8 | 0.16 |
| (1,221) | 1:2:A:GLY:H | 1:45:A:SER:HA | 8 | 0.16 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 12 | 0.16 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 17 | 0.16 |
| (1,160) | 1:30:A:THR:HG21 | 1:35:A:LEU:H | 14 | 0.16 |
| (1,160) | 1:30:A:THR:HG22 | 1:35:A:LEU:H | 14 | 0.16 |
| (1,160) | 1:30:A:THR:HG23 | 1:35:A:LEU:H | 14 | 0.16 |
| (1,123) | 1:31:A:LEU:H | 1:31:A:LEU:HG | 5 | 0.16 |
| (1,106) | 1:27:A:ASN:H | 1:27:A:ASN:HD21 | 20 | 0.16 |
| (1,106) | 1:27:A:ASN:H | 1:27:A:ASN:HD22 | 20 | 0.16 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 18 | 0.15 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 18 | 0.15 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 17 | 0.15 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 17 | 0.15 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 17 | 0.15 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 17 | 0.15 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 17 | 0.15 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 17 | 0.15 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD1 | 12 | 0.15 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD2 | 12 | 0.15 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD1 | 12 | 0.15 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD2 | 12 | 0.15 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD1 | 12 | 0.15 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD2 | 12 | 0.15 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE1 | 19 | 0.15 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE2 | 19 | 0.15 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE1 | 19 | 0.15 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE2 | 19 | 0.15 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE1 | 19 | 0.15 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE2 | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3844) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 15 | 0.15 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG11 | 1 | 0.15 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG12 | 1 | 0.15 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG13 | 1 | 0.15 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG21 | 1 | 0.15 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG22 | 1 | 0.15 |
| (1,3679) | 1:70:A:ALA:HB3 | 1:61:A:VAL:HG23 | 1 | 0.15 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 1 | 0.15 |
| (1,3672) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 1 | 0.15 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 9 | 0.15 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 9 | 0.15 |
| (1,3655) | 1:87:A:ALA:HB2 | 1:39:A:VAL:HA | 17 | 0.15 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB2 | 17 | 0.15 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB3 | 17 | 0.15 |
| (1,3649) | 1:129:A:ILE:HG23 | 1:131:A:VAL:H | 8 | 0.15 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 16 | 0.15 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 16 | 0.15 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 16 | 0.15 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 16 | 0.15 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 16 | 0.15 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 16 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD22 | 1:49:A:GLN:HB2 | 5 | 0.15 |
| (1,3545) | 1:55:A:LEU:HD22 | 1:49:A:GLN:HB3 | 5 | 0.15 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 10 | 0.15 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 10 | 0.15 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 15 | 0.15 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 15 | 0.15 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 10 | 0.15 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 10 | 0.15 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 10 | 0.15 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 10 | 0.15 |
| (1,3515) | 1:31:A:LEU:HD22 | 1:31:A:LEU:HA | 13 | 0.15 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB2 | 15 | 0.15 |
| (1,3490) | 1:17:A:LEU:HD13 | 1:20:A:ARG:HB3 | 15 | 0.15 |
| (1,3464) | 1:126:A:GLY:HA3 | 1:123:A:ALA:HA | 17 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD11 | 1 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD12 | 1 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD13 | 1 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD21 | 1 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD22 | 1 | 0.15 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD23 | 1 | 0.15 |
| (1,3421) | 1:22:A:ALA:HA | 1:191:A:PRO:HD2 | 18 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3421) | 1:22:A:ALA:HA | 1:191:A:PRO:HD3 | 18 | 0.15 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB1 | 5 | 0.15 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB2 | 5 | 0.15 |
| (1,3407) | 1:113:A:LEU:HB3 | 1:9:A:ALA:HB3 | 5 | 0.15 |
| (1,3398) | 1:71:A:VAL:H | 1:68:A:ARG:HA | 10 | 0.15 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA2 | 12 | 0.15 |
| (1,3382) | 1:187:A:GLY:H | 1:184:A:GLY:HA3 | 12 | 0.15 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB1 | 12 | 0.15 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB2 | 12 | 0.15 |
| (1,3368) | 1:74:A:VAL:H | 1:70:A:ALA:HB3 | 12 | 0.15 |
| (1,3355) | 1:28:A:THR:HG22 | 1:34:A:VAL:HB | 2 | 0.15 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 5 | 0.15 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 5 | 0.15 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 7 | 0.15 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 7 | 0.15 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 10 | 0.15 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 10 | 0.15 |
| (1,3210) | 1:185:A:PRO:HD2 | 1:199:A:GLY:HA2 | 17 | 0.15 |
| (1,3210) | 1:185:A:PRO:HD2 | 1:199:A:GLY:HA3 | 17 | 0.15 |
| (1,3210) | 1:185:A:PRO:HD3 | 1:199:A:GLY:HA2 | 17 | 0.15 |
| (1,3210) | 1:185:A:PRO:HD3 | 1:199:A:GLY:HA3 | 17 | 0.15 |
| (1,3208) | 1:99:A:VAL:HA | 1:197:A:PHE:HA | 17 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HA | 3 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 3 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 3 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HA | 3 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HA | 3 | 0.15 |
| (1,3202) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HA | 3 | 0.15 |
| (1,3197) | 1:191:A:PRO:HD2 | 1:194:A:GLN:HG2 | 8 | 0.15 |
| (1,3197) | 1:191:A:PRO:HD2 | 1:194:A:GLN:HG3 | 8 | 0.15 |
| (1,3197) | 1:191:A:PRO:HD3 | 1:194:A:GLN:HG2 | 8 | 0.15 |
| (1,3197) | 1:191:A:PRO:HD3 | 1:194:A:GLN:HG3 | 8 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD2 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD3 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD2 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD3 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD2 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD3 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD2 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD3 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD2 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD3 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD2 | 7 | 0.15 |
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD3 | 7 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG21 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG22 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG23 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG21 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG22 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG23 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG21 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG22 | 20 | 0.15 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG23 | 20 | 0.15 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB2 | 9 | 0.15 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB3 | 9 | 0.15 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB2 | 11 | 0.15 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB3 | 11 | 0.15 |
| (1,3060) | 1:137:A:GLN:HG2 | 1:141:A:SER:HA | 15 | 0.15 |
| (1,3060) | 1:137:A:GLN:HG3 | 1:141:A:SER:HA | 15 | 0.15 |
| (1,3052) | 1:29:A:SER:HB2 | 1:140:A:ILE:HA | 19 | 0.15 |
| (1,3052) | 1:29:A:SER:HB3 | 1:140:A:ILE:HA | 19 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG11 | 1:136:A:VAL:HB | 4 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG12 | 1:136:A:VAL:HB | 4 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG13 | 1:136:A:VAL:HB | 4 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG21 | 1:136:A:VAL:HB | 4 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG22 | 1:136:A:VAL:HB | 4 | 0.15 |
| (1,3003) | 1:131:A:VAL:HG23 | 1:136:A:VAL:HB | 4 | 0.15 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA2 | 14 | 0.15 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA3 | 14 | 0.15 |
| (1,2962) | 1:52:A:ALA:HB1 | 1:130:A:ASN:HB2 | 6 | 0.15 |
| (1,2962) | 1:52:A:ALA:HB1 | 1:130:A:ASN:HB3 | 6 | 0.15 |
| (1,2962) | 1:52:A:ALA:HB2 | 1:130:A:ASN:HB2 | 6 | 0.15 |
| (1,2962) | 1:52:A:ALA:HB2 | 1:130:A:ASN:HB3 | 6 | 0.15 |
| (1,2962) | 1:52:A:ALA:HB3 | 1:130:A:ASN:HB2 | 6 | 0.15 |
| (1,2962) | 1:52:A:ALA:HB3 | 1:130:A:ASN:HB3 | 6 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB2 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB3 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB2 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB3 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB2 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB3 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB2 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB3 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB2 | 8 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB3 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB2 | 8 | 0.15 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB3 | 8 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 9 | 0.15 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 9 | 0.15 |
| (1,2869) | 1:55:A:LEU:HB2 | 1:120:A:VAL:HA | 3 | 0.15 |
| (1,2869) | 1:55:A:LEU:HB3 | 1:120:A:VAL:HA | 3 | 0.15 |
| (1,2804) | 1:9:A:ALA:HB1 | 1:116:A:LEU:HB2 | 10 | 0.15 |
| (1,2804) | 1:9:A:ALA:HB1 | 1:116:A:LEU:HB3 | 10 | 0.15 |
| (1,2804) | 1:9:A:ALA:HB2 | 1:116:A:LEU:HB2 | 10 | 0.15 |
| (1,2804) | 1:9:A:ALA:HB2 | 1:116:A:LEU:HB3 | 10 | 0.15 |
| (1,2804) | 1:9:A:ALA:HB3 | 1:116:A:LEU:HB2 | 10 | 0.15 |
| (1,2804) | 1:9:A:ALA:HB3 | 1:116:A:LEU:HB3 | 10 | 0.15 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD11 | 8 | 0.15 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD12 | 8 | 0.15 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD13 | 8 | 0.15 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD21 | 8 | 0.15 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD22 | 8 | 0.15 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD23 | 8 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 13 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 13 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 13 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 13 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 13 | 0.15 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 13 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 14 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 6 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 14 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 14 | 0.15 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 14 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA2 | 1:99:A:VAL:HG11 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA2 | 1:99:A:VAL:HG12 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA2 | 1:99:A:VAL:HG13 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA2 | 1:99:A:VAL:HG21 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA2 | 1:99:A:VAL:HG22 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA2 | 1:99:A:VAL:HG23 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA3 | 1:99:A:VAL:HG11 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA3 | 1:99:A:VAL:HG12 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA3 | 1:99:A:VAL:HG13 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA3 | 1:99:A:VAL:HG21 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA3 | 1:99:A:VAL:HG22 | 15 | 0.15 |
| (1,2619) | 1:98:A:GLY:HA3 | 1:99:A:VAL:HG23 | 15 | 0.15 |
| (1,2609) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HA | 5 | 0.15 |
| (1,2609) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HA | 5 | 0.15 |
| (1,2609) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HA | 10 | 0.15 |
| (1,2609) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HA | 10 | 0.15 |
| (1,2609) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HA | 12 | 0.15 |
| (1,2609) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HA | 12 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 12 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 12 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 12 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 12 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 12 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 12 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 13 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 13 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 13 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 13 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 13 | 0.15 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 13 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE1 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE2 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE1 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE2 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE1 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE2 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE1 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE2 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE1 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE2 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE1 | 14 | 0.15 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE2 | 14 | 0.15 |
| (1,2432) | 1:44:A:ALA:HA | 1:77:A:LEU:HD11 | 3 | 0.15 |
| (1,2432) | 1:44:A:ALA:HA | 1:77:A:LEU:HD12 | 3 | 0.15 |
| (1,2432) | 1:44:A:ALA:HA | 1:77:A:LEU:HD13 | 3 | 0.15 |
| (1,2432) | 1:44:A:ALA:HA | 1:77:A:LEU:HD21 | 3 | 0.15 |
| (1,2432) | 1:44:A:ALA:HA | 1:77:A:LEU:HD22 | 3 | 0.15 |
| (1,2432) | 1:44:A:ALA:HA | 1:77:A:LEU:HD23 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB1 | 1:77:A:LEU:HD11 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB1 | 1:77:A:LEU:HD12 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB1 | 1:77:A:LEU:HD13 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB1 | 1:77:A:LEU:HD21 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB1 | 1:77:A:LEU:HD22 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB1 | 1:77:A:LEU:HD23 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB2 | 1:77:A:LEU:HD11 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB2 | 1:77:A:LEU:HD12 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB2 | 1:77:A:LEU:HD13 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB2 | 1:77:A:LEU:HD21 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB2 | 1:77:A:LEU:HD22 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB2 | 1:77:A:LEU:HD23 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB3 | 1:77:A:LEU:HD11 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB3 | 1:77:A:LEU:HD12 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB3 | 1:77:A:LEU:HD13 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB3 | 1:77:A:LEU:HD21 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB3 | 1:77:A:LEU:HD22 | 3 | 0.15 |
| (1,2429) | 1:73:A:ALA:HB3 | 1:77:A:LEU:HD23 | 3 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 16 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 16 | 0.15 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 16 | 0.15 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD2 | 15 | 0.15 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD3 | 15 | 0.15 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 6 | 0.15 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 6 | 0.15 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 6 | 0.15 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 6 | 0.15 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 6 | 0.15 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 6 | 0.15 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD21 | 7 | 0.15 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD22 | 7 | 0.15 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD21 | 7 | 0.15 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD22 | 7 | 0.15 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 19 | 0.15 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 19 | 0.15 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 19 | 0.15 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 20 | 0.15 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 20 | 0.15 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 20 | 0.15 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB2 | 6 | 0.15 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB3 | 6 | 0.15 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 7 | 0.15 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 7 | 0.15 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 17 | 0.15 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 17 | 0.15 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 8 | 0.15 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 8 | 0.15 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 9 | 0.15 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 9 | 0.15 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 11 | 0.15 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 11 | 0.15 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 16 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 16 | 0.15 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD11 | 10 | 0.15 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD12 | 10 | 0.15 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD13 | 10 | 0.15 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD11 | 10 | 0.15 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD12 | 10 | 0.15 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD13 | 10 | 0.15 |
| (1,1989) | 1:33:A:THR:HB | 1:34:A:VAL:H | 20 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD11 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD12 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD13 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD21 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD22 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD23 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD11 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD12 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD13 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD21 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD23 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD11 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD12 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD13 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD21 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD22 | 7 | 0.15 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD23 | 7 | 0.15 |
| (1,1803) | 1:177:A:THR:H | 1:175:A:PRO:HA | 1 | 0.15 |
| (1,1803) | 1:177:A:THR:H | 1:175:A:PRO:HA | 10 | 0.15 |
| (1,1660) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 2 | 0.15 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 1 | 0.15 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 7 | 0.15 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 17 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 15 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 15 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 15 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 15 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 15 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 15 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 20 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 20 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 20 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 20 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 20 | 0.15 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 20 | 0.15 |
| (1,1281) | 1:33:A:THR:HB | 1:34:A:VAL:H | 20 | 0.15 |
| (1,1177) | 1:108:A:LEU:H | 1:108:A:LEU:HG | 7 | 0.15 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG11 | 5 | 0.15 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG12 | 5 | 0.15 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG13 | 5 | 0.15 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG21 | 5 | 0.15 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG22 | 5 | 0.15 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG23 | 5 | 0.15 |
| (1,1151) | 1:131:A:VAL:H | 1:130:A:ASN:H | 13 | 0.15 |
| (1,1138) | 1:147:A:LEU:HB2 | 1:149:A:THR:H | 3 | 0.15 |
| (1,1138) | 1:76:A:ARG:HB2 | 1:74:A:VAL:H | 6 | 0.15 |
| (1,1138) | 1:76:A:ARG:HB3 | 1:74:A:VAL:H | 18 | 0.15 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG21 | 7 | 0.15 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG22 | 7 | 0.15 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG23 | 7 | 0.15 |
| (1,1127) | 1:163:A:SER:H | 1:162:A:SER:HA | 4 | 0.15 |
| (1,1123) | 1:132:A:ASP:H | 1:136:A:VAL:HB | 8 | 0.15 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD11 | 20 | 0.15 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD12 | 20 | 0.15 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD13 | 20 | 0.15 |
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 5 | 0.15 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 12 | 0.15 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 12 | 0.15 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 12 | 0.15 |
| (1,1053) | 1:34:A:VAL:H | 1:29:A:SER:HA | 20 | 0.15 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 1 | 0.15 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 1 | 0.15 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 1 | 0.15 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 1 | 0.15 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 1 | 0.15 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 1 | 0.15 |
| (1,1031) | 1:167:A:ALA:HA | 1:169:A:TYR:H | 13 | 0.15 |
| (1,1023) | 1:164:A:THR:HA | 1:166:A:GLY:H | 2 | 0.15 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 15 | 0.15 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 15 | 0.15 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 5 | 0.15 |
| (1,956) | 1:70:A:ALA:H | 1:68:A:ARG:H | 11 | 0.15 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA2 | 15 | 0.15 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA3 | 15 | 0.15 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG2 | 18 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG3 | 18 | 0.15 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB2 | 14 | 0.15 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB3 | 14 | 0.15 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 7 | 0.15 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 7 | 0.15 |
| (1,801) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 2 | 0.15 |
| (1,778) | 1:128:A:GLY:H | 1:129:A:ILE:HG12 | 20 | 0.15 |
| (1,778) | 1:128:A:GLY:H | 1:129:A:ILE:HG13 | 20 | 0.15 |
| (1,728) | 1:116:A:LEU:H | 1:120:A:VAL:H | 20 | 0.15 |
| (1,711) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,711) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,711) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD21 | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,708) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD21 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD22 | 15 | 0.15 |
| (1,708) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD11 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD12 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD13 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD21 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD22 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD21 | 18 | 0.15 |
| (1,708) | 1:117:A:LEU:HD23 | 1:118:A:ASN:HD22 | 18 | 0.15 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB2 | 1 | 0.15 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB3 | 1 | 0.15 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB2 | 11 | 0.15 |
| (1,688) | 1:10:A:THR:H | 1:116:A:LEU:HB3 | 11 | 0.15 |
| (1,609) | 1:101:A:ASN:H | 1:105:A:ILE:H | 5 | 0.15 |
| (1,598) | 1:96:A:ASN:HD21 | 1:104:A:ASN:HD21 | 10 | 0.15 |
| (1,598) | 1:96:A:ASN:HD21 | 1:104:A:ASN:HD22 | 10 | 0.15 |
| (1,598) | 1:96:A:ASN:HD22 | 1:104:A:ASN:HD21 | 10 | 0.15 |
| (1,598) | 1:96:A:ASN:HD22 | 1:104:A:ASN:HD22 | 10 | 0.15 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD21 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD22 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD21 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD22 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD21 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD22 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD21 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD22 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD21 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD22 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD21 | 9 | 0.15 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD22 | 9 | 0.15 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD21 | 10 | 0.15 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD22 | 10 | 0.15 |
| (1,561) | 1:22:A:ALA:H | 1:100:A:LEU:HA | 16 | 0.15 |
| (1,524) | 1:37:A:THR:H | 1:95:A:PHE:HB2 | 1 | 0.15 |
| (1,524) | 1:37:A:THR:H | 1:95:A:PHE:HB3 | 1 | 0.15 |
| (1,455) | 1:83:A:THR:HG21 | 1:84:A:SER:H | 6 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,455) | 1:83:A:THR:HG22 | 1:84:A:SER:H | 6 | 0.15 |
| (1,455) | 1:83:A:THR:HG23 | 1:84:A:SER:H | 6 | 0.15 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 17 | 0.15 |
| (1,417) | 1:73:A:ALA:H | 1:76:A:ARG:HB2 | 8 | 0.15 |
| (1,417) | 1:73:A:ALA:H | 1:76:A:ARG:HB3 | 8 | 0.15 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD21 | 2 | 0.15 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD22 | 2 | 0.15 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD21 | 2 | 0.15 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD22 | 2 | 0.15 |
| (1,258) | 1:49:A:GLN:HB2 | 1:51:A:ALA:H | 20 | 0.15 |
| (1,258) | 1:49:A:GLN:HB3 | 1:51:A:ALA:H | 20 | 0.15 |
| (1,233) | 1:45:A:SER:HB2 | 1:47:A:VAL:H | 19 | 0.15 |
| (1,233) | 1:45:A:SER:HB3 | 1:47:A:VAL:H | 19 | 0.15 |
| (1,221) | 1:2:A:GLY:H | 1:45:A:SER:HA | 12 | 0.15 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 1 | 0.15 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 1 | 0.15 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 5 | 0.15 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 7 | 0.14 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 7 | 0.14 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 3 | 0.14 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 3 | 0.14 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE1 | 19 | 0.14 |
| (1,3909) | 1:74:A:VAL:HB | 1:86:A:TYR:HE2 | 19 | 0.14 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD1 | 13 | 0.14 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD2 | 13 | 0.14 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD1 | 13 | 0.14 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD2 | 13 | 0.14 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD1 | 13 | 0.14 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD2 | 13 | 0.14 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE1 | 6 | 0.14 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE2 | 6 | 0.14 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE1 | 6 | 0.14 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE2 | 6 | 0.14 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE1 | 6 | 0.14 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE2 | 6 | 0.14 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE1 | 15 | 0.14 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE2 | 15 | 0.14 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE1 | 15 | 0.14 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE2 | 15 | 0.14 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE1 | 15 | 0.14 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE2 | 15 | 0.14 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB2 | 19 | 0.14 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB3 | 19 | 0.14 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG21 | 18 | 0.14 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG22 | 18 | 0.14 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG23 | 18 | 0.14 |
| (1,3654) | 1:39:A:VAL:HG12 | 1:38:A:GLY:HA2 | 4 | 0.14 |
| (1,3654) | 1:39:A:VAL:HG12 | 1:38:A:GLY:HA3 | 4 | 0.14 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB2 | 11 | 0.14 |
| (1,3652) | 1:118:A:ASN:HD22 | 1:114:A:SER:HB3 | 11 | 0.14 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB2 | 11 | 0.14 |
| (1,3640) | 1:172:A:PRO:HB2 | 1:173:A:SER:HB3 | 11 | 0.14 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB2 | 12 | 0.14 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB3 | 12 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB1 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB2 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG11 | 1:22:A:ALA:HB3 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB1 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB2 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG12 | 1:22:A:ALA:HB3 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB1 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB2 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG13 | 1:22:A:ALA:HB3 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB1 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB2 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG21 | 1:22:A:ALA:HB3 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB1 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB2 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG22 | 1:22:A:ALA:HB3 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB1 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB2 | 14 | 0.14 |
| (1,3592) | 1:99:A:VAL:HG23 | 1:22:A:ALA:HB3 | 14 | 0.14 |
| (1,3545) | 1:55:A:LEU:HD23 | 1:49:A:GLN:HB2 | 7 | 0.14 |
| (1,3545) | 1:55:A:LEU:HD23 | 1:49:A:GLN:HB3 | 7 | 0.14 |
| (1,3543) | 1:17:A:LEU:HD13 | 1:93:A:ALA:HA | 6 | 0.14 |
| (1,3515) | 1:31:A:LEU:HD21 | 1:31:A:LEU:HA | 5 | 0.14 |
| (1,3502) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HG2 | 10 | 0.14 |
| (1,3502) | 1:39:A:VAL:HG22 | 1:36:A:ARG:HG3 | 10 | 0.14 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 8 | 0.14 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 8 | 0.14 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB2 | 17 | 0.14 |
| (1,3490) | 1:17:A:LEU:HD11 | 1:20:A:ARG:HB3 | 17 | 0.14 |
| (1,3473) | 1:21:A:VAL:HG11 | 1:92:A:SER:HA | 16 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3473) | 1:21:A:VAL:HG12 | 1:92:A:SER:HA | 16 | 0.14 |
| (1,3473) | 1:21:A:VAL:HG13 | 1:92:A:SER:HA | 16 | 0.14 |
| (1,3473) | 1:21:A:VAL:HG21 | 1:92:A:SER:HA | 16 | 0.14 |
| (1,3473) | 1:21:A:VAL:HG22 | 1:92:A:SER:HA | 16 | 0.14 |
| (1,3473) | 1:21:A:VAL:HG23 | 1:92:A:SER:HA | 16 | 0.14 |
| (1,3406) | 1:82:A:ASP:H | 1:82:A:ASP:HA | 8 | 0.14 |
| (1,3368) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 4 | 0.14 |
| (1,3368) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 4 | 0.14 |
| (1,3368) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 4 | 0.14 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 7 | 0.14 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 7 | 0.14 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD11 | 18 | 0.14 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD12 | 18 | 0.14 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD13 | 18 | 0.14 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD21 | 18 | 0.14 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD22 | 18 | 0.14 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD23 | 18 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 6 | 0.14 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 6 | 0.14 |
| (1,3268) | 1:10:A:THR:HA | 1:113:A:LEU:HG | 10 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA2 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA3 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA2 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA3 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA2 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA3 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA2 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA3 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA2 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA3 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA2 | 11 | 0.14 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA3 | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD2 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD3 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD2 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD3 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD2 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD3 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD2 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD3 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD2 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD3 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD2 | 4 | 0.14 |
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD3 | 4 | 0.14 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB1 | 1 | 0.14 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB2 | 1 | 0.14 |
| (1,3111) | 1:158:A:GLN:HA | 1:161:A:ALA:HB3 | 1 | 0.14 |
| (1,3105) | 1:156:A:TYR:HB2 | 1:158:A:GLN:HG2 | 6 | 0.14 |
| (1,3105) | 1:156:A:TYR:HB2 | 1:158:A:GLN:HG3 | 6 | 0.14 |
| (1,3105) | 1:156:A:TYR:HB3 | 1:158:A:GLN:HG2 | 6 | 0.14 |
| (1,3105) | 1:156:A:TYR:HB3 | 1:158:A:GLN:HG3 | 6 | 0.14 |
| (1,3104) | 1:156:A:TYR:HB2 | 1:158:A:GLN:HG2 | 6 | 0.14 |
| (1,3104) | 1:156:A:TYR:HB2 | 1:158:A:GLN:HG3 | 6 | 0.14 |
| (1,3104) | 1:156:A:TYR:HB3 | 1:158:A:GLN:HG2 | 6 | 0.14 |
| (1,3104) | 1:156:A:TYR:HB3 | 1:158:A:GLN:HG3 | 6 | 0.14 |
| (1,3095) | 1:146:A:PHE:HB2 | 1:150:A:SER:HA | 1 | 0.14 |
| (1,3095) | 1:146:A:PHE:HB3 | 1:150:A:SER:HA | 1 | 0.14 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG21 | 12 | 0.14 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG22 | 12 | 0.14 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG23 | 12 | 0.14 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG21 | 12 | 0.14 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG22 | 12 | 0.14 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG23 | 12 | 0.14 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB2 | 20 | 0.14 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB3 | 20 | 0.14 |
| (1,3021) | 1:28:A:THR:HG21 | 1:139:A:ASP:HA | 18 | 0.14 |
| (1,3021) | 1:28:A:THR:HG22 | 1:139:A:ASP:HA | 18 | 0.14 |
| (1,3021) | 1:28:A:THR:HG23 | 1:139:A:ASP:HA | 18 | 0.14 |
| (1,3005) | 1:37:A:THR:HG21 | 1:136:A:VAL:HA | 9 | 0.14 |
| (1,3005) | 1:37:A:THR:HG22 | 1:136:A:VAL:HA | 9 | 0.14 |
| (1,3005) | 1:37:A:THR:HG23 | 1:136:A:VAL:HA | 9 | 0.14 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB2 | 10 | 0.14 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB3 | 10 | 0.14 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB2 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB3 | 10 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB1 | 1:125:A:GLN:HG2 | 1 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB1 | 1:125:A:GLN:HG3 | 1 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HG2 | 1 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HG3 | 1 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HG2 | 1 | 0.14 |
| (1,2898) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HG3 | 1 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG11 | 1:124:A:ALA:HB1 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG11 | 1:124:A:ALA:HB2 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG11 | 1:124:A:ALA:HB3 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG12 | 1:124:A:ALA:HB1 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG12 | 1:124:A:ALA:HB2 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG12 | 1:124:A:ALA:HB3 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG13 | 1:124:A:ALA:HB1 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG13 | 1:124:A:ALA:HB2 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG13 | 1:124:A:ALA:HB3 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG21 | 1:124:A:ALA:HB1 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG21 | 1:124:A:ALA:HB2 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG21 | 1:124:A:ALA:HB3 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG22 | 1:124:A:ALA:HB1 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG22 | 1:124:A:ALA:HB2 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG22 | 1:124:A:ALA:HB3 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG23 | 1:124:A:ALA:HB1 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG23 | 1:124:A:ALA:HB2 | 13 | 0.14 |
| (1,2890) | 1:120:A:VAL:HG23 | 1:124:A:ALA:HB3 | 13 | 0.14 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD11 | 5 | 0.14 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD12 | 5 | 0.14 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD13 | 5 | 0.14 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD21 | 5 | 0.14 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD22 | 5 | 0.14 |
| (1,2805) | 1:36:A:ARG:HE | 1:116:A:LEU:HD23 | 5 | 0.14 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 2 | 0.14 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 2 | 0.14 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 3 | 0.14 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 3 | 0.14 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD2 | 9 | 0.14 |
| (1,2755) | 1:105:A:ILE:HA | 1:111:A:ARG:HD3 | 9 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 1 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 1 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 1 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 1 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 2 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 2 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 2 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 10 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 10 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 10 | 0.14 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 10 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 9 | 0.14 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 9 | 0.14 |
| (1,2720) | 1:107:A:THR:HG21 | 1:108:A:LEU:HB2 | 15 | 0.14 |
| (1,2720) | 1:107:A:THR:HG21 | 1:108:A:LEU:HB3 | 15 | 0.14 |
| (1,2720) | 1:107:A:THR:HG22 | 1:108:A:LEU:HB2 | 15 | 0.14 |
| (1,2720) | 1:107:A:THR:HG22 | 1:108:A:LEU:HB3 | 15 | 0.14 |
| (1,2720) | 1:107:A:THR:HG23 | 1:108:A:LEU:HB2 | 15 | 0.14 |
| (1,2720) | 1:107:A:THR:HG23 | 1:108:A:LEU:HB3 | 15 | 0.14 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB2 | 11 | 0.14 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB3 | 11 | 0.14 |
| (1,2520) | 1:85:A:ALA:HA | 1:88:A:GLN:HB2 | 11 | 0.14 |
| (1,2520) | 1:85:A:ALA:HA | 1:88:A:GLN:HB3 | 11 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD1 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD11 | 1:86:A:TYR:HD2 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD1 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD12 | 1:86:A:TYR:HD2 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD1 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HD2 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD1 | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2496) | 1:35:A:LEU:HD21 | 1:86:A:TYR:HD2 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD1 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD22 | 1:86:A:TYR:HD2 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD1 | 6 | 0.14 |
| (1,2496) | 1:35:A:LEU:HD23 | 1:86:A:TYR:HD2 | 6 | 0.14 |
| (1,2492) | 1:77:A:LEU:HD11 | 1:86:A:TYR:HA | 8 | 0.14 |
| (1,2492) | 1:77:A:LEU:HD12 | 1:86:A:TYR:HA | 8 | 0.14 |
| (1,2492) | 1:77:A:LEU:HD13 | 1:86:A:TYR:HA | 8 | 0.14 |
| (1,2492) | 1:77:A:LEU:HD21 | 1:86:A:TYR:HA | 8 | 0.14 |
| (1,2492) | 1:77:A:LEU:HD22 | 1:86:A:TYR:HA | 8 | 0.14 |
| (1,2492) | 1:77:A:LEU:HD23 | 1:86:A:TYR:HA | 8 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE1 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE2 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE1 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE2 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE1 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE2 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE1 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE2 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE1 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE2 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE1 | 12 | 0.14 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE2 | 12 | 0.14 |
| (1,2427) | 1:74:A:VAL:HB | 1:77:A:LEU:HD11 | 20 | 0.14 |
| (1,2427) | 1:74:A:VAL:HB | 1:77:A:LEU:HD12 | 20 | 0.14 |
| (1,2427) | 1:74:A:VAL:HB | 1:77:A:LEU:HD13 | 20 | 0.14 |
| (1,2427) | 1:74:A:VAL:HB | 1:77:A:LEU:HD21 | 20 | 0.14 |
| (1,2427) | 1:74:A:VAL:HB | 1:77:A:LEU:HD22 | 20 | 0.14 |
| (1,2427) | 1:74:A:VAL:HB | 1:77:A:LEU:HD23 | 20 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 13 | 0.14 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 13 | 0.14 |
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD2 | 19 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2398) | 1:76:A:ARG:HA | 1:76:A:ARG:HD3 | 19 | 0.14 |
| (1,2272) | 1:48:A:VAL:HA | 1:65:A:ASN:HD21 | 19 | 0.14 |
| (1,2272) | 1:48:A:VAL:HA | 1:65:A:ASN:HD22 | 19 | 0.14 |
| (1,2241) | 1:58:A:THR:HG21 | 1:61:A:VAL:HB | 13 | 0.14 |
| (1,2241) | 1:58:A:THR:HG22 | 1:61:A:VAL:HB | 13 | 0.14 |
| (1,2241) | 1:58:A:THR:HG23 | 1:61:A:VAL:HB | 13 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG21 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG22 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG23 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG21 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG22 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG23 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG21 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG22 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG23 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG21 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG22 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG23 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG21 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG22 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG23 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG21 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG22 | 7 | 0.14 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG23 | 7 | 0.14 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 1 | 0.14 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 1 | 0.14 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 1 | 0.14 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB2 | 14 | 0.14 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB3 | 14 | 0.14 |
| (1,2205) | 1:49:A:GLN:HG2 | 1:56:A:ALA:HB1 | 10 | 0.14 |
| (1,2205) | 1:49:A:GLN:HG2 | 1:56:A:ALA:HB2 | 10 | 0.14 |
| (1,2205) | 1:49:A:GLN:HG2 | 1:56:A:ALA:HB3 | 10 | 0.14 |
| (1,2205) | 1:49:A:GLN:HG3 | 1:56:A:ALA:HB1 | 10 | 0.14 |
| (1,2205) | 1:49:A:GLN:HG3 | 1:56:A:ALA:HB2 | 10 | 0.14 |
| (1,2205) | 1:49:A:GLN:HG3 | 1:56:A:ALA:HB3 | 10 | 0.14 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 20 | 0.14 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 20 | 0.14 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 11 | 0.14 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 11 | 0.14 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 13 | 0.14 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 13 | 0.14 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 14 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 14 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG21 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG22 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG23 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG21 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG22 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG23 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG21 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG22 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG23 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG21 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG22 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG23 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG21 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG22 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG23 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG21 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG22 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG23 | 1 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG21 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG22 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG23 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG21 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG22 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG23 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG21 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG22 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG23 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG21 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG22 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG23 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG21 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG22 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG23 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG21 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG22 | 18 | 0.14 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG23 | 18 | 0.14 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD11 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD12 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD13 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD21 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD22 | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD23 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD11 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD12 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD13 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD21 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD23 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD11 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD12 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD13 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD21 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD22 | 11 | 0.14 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD23 | 11 | 0.14 |
| (1,1904) | 1:20:A:ARG:HA | 1:24:A:ALA:HA | 1 | 0.14 |
| (1,1660) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 8 | 0.14 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 13 | 0.14 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 15 | 0.14 |
| (1,1551) | 1:99:A:VAL:HB | 1:100:A:LEU:H | 15 | 0.14 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 11 | 0.14 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 19 | 0.14 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 16 | 0.14 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 16 | 0.14 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 16 | 0.14 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 16 | 0.14 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 16 | 0.14 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 16 | 0.14 |
| (1,1403) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 7 | 0.14 |
| (1,1403) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 7 | 0.14 |
| (1,1401) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 10 | 0.14 |
| (1,1401) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 10 | 0.14 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD2 | 9 | 0.14 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 9 | 0.14 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 20 | 0.14 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 20 | 0.14 |
| (1,1148) | 1:134:A:GLY:H | 1:67:A:ALA:HA | 13 | 0.14 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB2 | 17 | 0.14 |
| (1,1148) | 1:134:A:GLY:H | 1:135:A:SER:HB3 | 17 | 0.14 |
| (1,1143) | 1:127:A:LEU:H | 1:123:A:ALA:HB1 | 12 | 0.14 |
| (1,1143) | 1:127:A:LEU:H | 1:123:A:ALA:HB2 | 12 | 0.14 |
| (1,1143) | 1:127:A:LEU:H | 1:123:A:ALA:HB3 | 12 | 0.14 |
| (1,1138) | 1:76:A:ARG:HB3 | 1:74:A:VAL:H | 5 | 0.14 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG21 | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|------------------|----------|---------------|
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG22 | 2 | 0.14 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG23 | 2 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 1 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 2 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 7 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 8 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 14 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 16 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 17 | 0.14 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 20 | 0.14 |
| (1,1123) | 1:132:A:ASP:H | 1:136:A:VAL:HB | 7 | 0.14 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB1 | 4 | 0.14 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB2 | 4 | 0.14 |
| (1,1114) | 1:69:A:PHE:H | 1:70:A:ALA:HB3 | 4 | 0.14 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 6 | 0.14 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 11 | 0.14 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 18 | 0.14 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 19 | 0.14 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 19 | 0.14 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 19 | 0.14 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 19 | 0.14 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 19 | 0.14 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 19 | 0.14 |
| (1,1015) | 1:17:A:LEU:H | 1:14:A:SER:H | 5 | 0.14 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 6 | 0.14 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 6 | 0.14 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG11 | 9 | 0.14 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG12 | 9 | 0.14 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG13 | 9 | 0.14 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG21 | 9 | 0.14 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG22 | 9 | 0.14 |
| (1,988) | 1:23:A:ASN:H | 1:21:A:VAL:HG23 | 9 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 10 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 10 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 10 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 10 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 10 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 10 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 16 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 16 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 16 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 16 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 16 | 0.14 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 16 | 0.14 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA2 | 9 | 0.14 |
| (1,953) | 1:121:A:SER:H | 1:119:A:GLY:HA3 | 9 | 0.14 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA2 | 14 | 0.14 |
| (1,952) | 1:104:A:ASN:HD22 | 1:109:A:GLY:HA3 | 14 | 0.14 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB2 | 13 | 0.14 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB3 | 13 | 0.14 |
| (1,928) | 1:178:A:GLY:HA2 | 1:187:A:GLY:H | 3 | 0.14 |
| (1,928) | 1:178:A:GLY:HA3 | 1:187:A:GLY:H | 3 | 0.14 |
| (1,927) | 1:179:A:PRO:HD2 | 1:187:A:GLY:H | 11 | 0.14 |
| (1,927) | 1:179:A:PRO:HD3 | 1:187:A:GLY:H | 11 | 0.14 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 18 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB2 | 5 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB3 | 5 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB2 | 18 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB3 | 18 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB2 | 20 | 0.14 |
| (1,899) | 1:162:A:SER:H | 1:162:A:SER:HB3 | 20 | 0.14 |
| (1,892) | 1:153:A:SER:H | 1:158:A:GLN:HB2 | 3 | 0.14 |
| (1,892) | 1:153:A:SER:H | 1:158:A:GLN:HB3 | 3 | 0.14 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB2 | 13 | 0.14 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB3 | 13 | 0.14 |
| (1,876) | 1:148:A:SER:H | 1:149:A:THR:H | 13 | 0.14 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 2 | 0.14 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 2 | 0.14 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 5 | 0.14 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 5 | 0.14 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 11 | 0.14 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 11 | 0.14 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 18 | 0.14 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 18 | 0.14 |
| (1,809) | 1:67:A:ALA:HB1 | 1:134:A:GLY:H | 19 | 0.14 |
| (1,809) | 1:67:A:ALA:HB2 | 1:134:A:GLY:H | 19 | 0.14 |
| (1,809) | 1:67:A:ALA:HB3 | 1:134:A:GLY:H | 19 | 0.14 |
| (1,801) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 8 | 0.14 |
| (1,778) | 1:128:A:GLY:H | 1:129:A:ILE:HG12 | 14 | 0.14 |
| (1,778) | 1:128:A:GLY:H | 1:129:A:ILE:HG13 | 14 | 0.14 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD21 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD22 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD21 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD22 | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD21 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD22 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD21 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD22 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD21 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD22 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD21 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD22 | 10 | 0.14 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD21 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD22 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD21 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD22 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD21 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD22 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD21 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD22 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD21 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD22 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD21 | 18 | 0.14 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD22 | 18 | 0.14 |
| (1,589) | 1:101:A:ASN:H | 1:104:A:ASN:H | 10 | 0.14 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD21 | 7 | 0.14 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD22 | 7 | 0.14 |
| (1,559) | 1:99:A:VAL:HB | 1:100:A:LEU:H | 15 | 0.14 |
| (1,455) | 1:83:A:THR:HG21 | 1:84:A:SER:H | 7 | 0.14 |
| (1,455) | 1:83:A:THR:HG22 | 1:84:A:SER:H | 7 | 0.14 |
| (1,455) | 1:83:A:THR:HG23 | 1:84:A:SER:H | 7 | 0.14 |
| (1,438) | 1:80:A:GLY:H | 1:81:A:SER:HB2 | 20 | 0.14 |
| (1,438) | 1:80:A:GLY:H | 1:81:A:SER:HB3 | 20 | 0.14 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 11 | 0.14 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 19 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG11 | 8 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG12 | 8 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG13 | 8 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG21 | 8 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG22 | 8 | 0.14 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG23 | 8 | 0.14 |
| (1,315) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 7 | 0.14 |
| (1,315) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 7 | 0.14 |
| (1,313) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 10 | 0.14 |
| (1,313) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 10 | 0.14 |
| (1,312) | 1:59:A:LEU:HB2 | 1:61:A:VAL:H | 10 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,312) | 1:59:A:LEU:HB3 | 1:61:A:VAL:H | 10 | 0.14 |
| (1,295) | 1:50:A:ARG:HB2 | 1:57:A:SER:H | 6 | 0.14 |
| (1,295) | 1:50:A:ARG:HB3 | 1:57:A:SER:H | 6 | 0.14 |
| (1,221) | 1:2:A:GLY:H | 1:45:A:SER:HA | 4 | 0.14 |
| (1,221) | 1:2:A:GLY:H | 1:45:A:SER:HA | 15 | 0.14 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 20 | 0.14 |
| (1,23) | 1:11:A:GLY:HA2 | 1:14:A:SER:H | 6 | 0.14 |
| (1,23) | 1:11:A:GLY:HA3 | 1:14:A:SER:H | 6 | 0.14 |
| (1,11) | 1:4:A:GLN:H | 1:8:A:GLY:H | 20 | 0.14 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD1 | 16 | 0.13 |
| (1,3910) | 1:85:A:ALA:HA | 1:86:A:TYR:HD2 | 16 | 0.13 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 2 | 0.13 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 2 | 0.13 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 2 | 0.13 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 2 | 0.13 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 2 | 0.13 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 2 | 0.13 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE1 | 4 | 0.13 |
| (1,3906) | 1:30:A:THR:HG21 | 1:95:A:PHE:HE2 | 4 | 0.13 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE1 | 4 | 0.13 |
| (1,3906) | 1:30:A:THR:HG22 | 1:95:A:PHE:HE2 | 4 | 0.13 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE1 | 4 | 0.13 |
| (1,3906) | 1:30:A:THR:HG23 | 1:95:A:PHE:HE2 | 4 | 0.13 |
| (1,3876) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 13 | 0.13 |
| (1,3876) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 13 | 0.13 |
| (1,3876) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 13 | 0.13 |
| (1,3876) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 13 | 0.13 |
| (1,3876) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 13 | 0.13 |
| (1,3876) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 13 | 0.13 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 2 | 0.13 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 9 | 0.13 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 17 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD11 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD12 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD13 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD21 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD22 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB1 | 1:77:A:LEU:HD23 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD11 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD12 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD13 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD21 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD22 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB2 | 1:77:A:LEU:HD23 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD11 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD12 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD13 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD21 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD22 | 13 | 0.13 |
| (1,3854) | 1:85:A:ALA:HB3 | 1:77:A:LEU:HD23 | 13 | 0.13 |
| (1,3796) | 1:124:A:ALA:HB2 | 1:120:A:VAL:HA | 11 | 0.13 |
| (1,3790) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 1 | 0.13 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB2 | 11 | 0.13 |
| (1,3763) | 1:41:A:GLN:HB2 | 1:45:A:SER:HB3 | 11 | 0.13 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB2 | 17 | 0.13 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB3 | 17 | 0.13 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG2 | 11 | 0.13 |
| (1,3718) | 1:18:A:ILE:HG12 | 1:20:A:ARG:HG3 | 11 | 0.13 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG2 | 11 | 0.13 |
| (1,3718) | 1:18:A:ILE:HG13 | 1:20:A:ARG:HG3 | 11 | 0.13 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG11 | 3 | 0.13 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG12 | 3 | 0.13 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG13 | 3 | 0.13 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG21 | 3 | 0.13 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG22 | 3 | 0.13 |
| (1,3679) | 1:70:A:ALA:HB2 | 1:61:A:VAL:HG23 | 3 | 0.13 |
| (1,3620) | 1:166:A:GLY:HA2 | 1:163:A:SER:HA | 4 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD11 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD12 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD13 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD21 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD22 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD23 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD11 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD12 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD13 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD21 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD22 | 10 | 0.13 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD23 | 10 | 0.13 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD11 | 14 | 0.13 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD12 | 14 | 0.13 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD13 | 14 | 0.13 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD21 | 14 | 0.13 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD22 | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD23 | 14 | 0.13 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD11 | 14 | 0.13 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD12 | 14 | 0.13 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD13 | 14 | 0.13 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD21 | 14 | 0.13 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD22 | 14 | 0.13 |
| (1,3472) | 1:117:A:LEU:HB2 | 1:113:A:LEU:HD23 | 14 | 0.13 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG11 | 10 | 0.13 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG12 | 10 | 0.13 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG13 | 10 | 0.13 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG21 | 10 | 0.13 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG22 | 10 | 0.13 |
| (1,3454) | 1:35:A:LEU:HD13 | 1:34:A:VAL:HG23 | 10 | 0.13 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG2 | 4 | 0.13 |
| (1,3437) | 1:101:A:ASN:HB2 | 1:194:A:GLN:HG3 | 4 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD11 | 6 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD12 | 6 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD13 | 6 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD21 | 6 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD22 | 6 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD23 | 6 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD11 | 20 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD12 | 20 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD13 | 20 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD21 | 20 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD22 | 20 | 0.13 |
| (1,3424) | 1:27:A:ASN:HB2 | 1:25:A:LEU:HD23 | 20 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB2 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD11 | 1:195:A:SER:HB3 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB2 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD12 | 1:195:A:SER:HB3 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB2 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD13 | 1:195:A:SER:HB3 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB2 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD21 | 1:195:A:SER:HB3 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB2 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD22 | 1:195:A:SER:HB3 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB2 | 13 | 0.13 |
| (1,3413) | 1:100:A:LEU:HD23 | 1:195:A:SER:HB3 | 13 | 0.13 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD2 | 2 | 0.13 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD3 | 2 | 0.13 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD11 | 1 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD12 | 1 | 0.13 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD13 | 1 | 0.13 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD21 | 1 | 0.13 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD22 | 1 | 0.13 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD23 | 1 | 0.13 |
| (1,3285) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE1 | 13 | 0.13 |
| (1,3285) | 1:44:A:ALA:HB1 | 1:86:A:TYR:HE2 | 13 | 0.13 |
| (1,3285) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE1 | 13 | 0.13 |
| (1,3285) | 1:44:A:ALA:HB2 | 1:86:A:TYR:HE2 | 13 | 0.13 |
| (1,3285) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE1 | 13 | 0.13 |
| (1,3285) | 1:44:A:ALA:HB3 | 1:86:A:TYR:HE2 | 13 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 17 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 17 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 17 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 17 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 17 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 17 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 20 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 20 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 20 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 20 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 20 | 0.13 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 20 | 0.13 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG2 | 7 | 0.13 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG3 | 7 | 0.13 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG2 | 7 | 0.13 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG3 | 7 | 0.13 |
| (1,3202) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HA | 19 | 0.13 |
| (1,3202) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HA | 19 | 0.13 |
| (1,3202) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HA | 19 | 0.13 |
| (1,3202) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HA | 19 | 0.13 |
| (1,3202) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HA | 19 | 0.13 |
| (1,3202) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HA | 19 | 0.13 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 14 | 0.13 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 14 | 0.13 |
| (1,3171) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HA | 1 | 0.13 |
| (1,3171) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HA | 1 | 0.13 |
| (1,3169) | 1:178:A:GLY:HA2 | 1:190:A:ALA:HA | 1 | 0.13 |
| (1,3169) | 1:178:A:GLY:HA3 | 1:190:A:ALA:HA | 1 | 0.13 |
| (1,3166) | 1:186:A:LEU:HD11 | 1:190:A:ALA:H | 4 | 0.13 |
| (1,3166) | 1:186:A:LEU:HD12 | 1:190:A:ALA:H | 4 | 0.13 |
| (1,3166) | 1:186:A:LEU:HD13 | 1:190:A:ALA:H | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3166) | 1:186:A:LEU:HD21 | 1:190:A:ALA:H | 4 | 0.13 |
| (1,3166) | 1:186:A:LEU:HD22 | 1:190:A:ALA:H | 4 | 0.13 |
| (1,3166) | 1:186:A:LEU:HD23 | 1:190:A:ALA:H | 4 | 0.13 |
| (1,3121) | 1:170:A:THR:HB | 1:171:A:GLY:HA2 | 6 | 0.13 |
| (1,3121) | 1:170:A:THR:HB | 1:171:A:GLY:HA3 | 6 | 0.13 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG2 | 16 | 0.13 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG3 | 16 | 0.13 |
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG2 | 16 | 0.13 |
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG3 | 16 | 0.13 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB1 | 14 | 0.13 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB2 | 14 | 0.13 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB3 | 14 | 0.13 |
| (1,3095) | 1:146:A:PHE:HB2 | 1:150:A:SER:HA | 20 | 0.13 |
| (1,3095) | 1:146:A:PHE:HB3 | 1:150:A:SER:HA | 20 | 0.13 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG21 | 14 | 0.13 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG22 | 14 | 0.13 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG23 | 14 | 0.13 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG21 | 14 | 0.13 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG22 | 14 | 0.13 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG23 | 14 | 0.13 |
| (1,3060) | 1:137:A:GLN:HG2 | 1:141:A:SER:HA | 6 | 0.13 |
| (1,3060) | 1:137:A:GLN:HG3 | 1:141:A:SER:HA | 6 | 0.13 |
| (1,3021) | 1:28:A:THR:HG21 | 1:139:A:ASP:HA | 10 | 0.13 |
| (1,3021) | 1:28:A:THR:HG22 | 1:139:A:ASP:HA | 10 | 0.13 |
| (1,3021) | 1:28:A:THR:HG23 | 1:139:A:ASP:HA | 10 | 0.13 |
| (1,3005) | 1:37:A:THR:HG21 | 1:136:A:VAL:HA | 19 | 0.13 |
| (1,3005) | 1:37:A:THR:HG22 | 1:136:A:VAL:HA | 19 | 0.13 |
| (1,3005) | 1:37:A:THR:HG23 | 1:136:A:VAL:HA | 19 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 13 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 16 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 16 | 0.13 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 16 | 0.13 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB2 | 4 | 0.13 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB3 | 4 | 0.13 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB2 | 4 | 0.13 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB3 | 4 | 0.13 |
| (1,2906) | 1:105:A:ILE:HG21 | 1:125:A:GLN:HG2 | 9 | 0.13 |
| (1,2906) | 1:105:A:ILE:HG21 | 1:125:A:GLN:HG3 | 9 | 0.13 |
| (1,2906) | 1:105:A:ILE:HG22 | 1:125:A:GLN:HG2 | 9 | 0.13 |
| (1,2906) | 1:105:A:ILE:HG22 | 1:125:A:GLN:HG3 | 9 | 0.13 |
| (1,2906) | 1:105:A:ILE:HG23 | 1:125:A:GLN:HG2 | 9 | 0.13 |
| (1,2906) | 1:105:A:ILE:HG23 | 1:125:A:GLN:HG3 | 9 | 0.13 |
| (1,2898) | 1:124:A:ALA:HB1 | 1:125:A:GLN:HG2 | 19 | 0.13 |
| (1,2898) | 1:124:A:ALA:HB1 | 1:125:A:GLN:HG3 | 19 | 0.13 |
| (1,2898) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HG2 | 19 | 0.13 |
| (1,2898) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HG3 | 19 | 0.13 |
| (1,2898) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HG2 | 19 | 0.13 |
| (1,2898) | 1:124:A:ALA:HB3 | 1:125:A:GLN:HG3 | 19 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB1 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB2 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD11 | 1:123:A:ALA:HB3 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB1 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB2 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD12 | 1:123:A:ALA:HB3 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB1 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB2 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD13 | 1:123:A:ALA:HB3 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB1 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB2 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD21 | 1:123:A:ALA:HB3 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB1 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB2 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD22 | 1:123:A:ALA:HB3 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB1 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB2 | 4 | 0.13 |
| (1,2884) | 1:55:A:LEU:HD23 | 1:123:A:ALA:HB3 | 4 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 10 | 0.13 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 10 | 0.13 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB2 | 8 | 0.13 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB3 | 8 | 0.13 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB1 | 11 | 0.13 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB2 | 11 | 0.13 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB3 | 11 | 0.13 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB1 | 11 | 0.13 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB2 | 11 | 0.13 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB3 | 11 | 0.13 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE21 | 18 | 0.13 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE22 | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE21 | 18 | 0.13 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE22 | 18 | 0.13 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE21 | 18 | 0.13 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE22 | 18 | 0.13 |
| (1,2492) | 1:77:A:LEU:HD11 | 1:86:A:TYR:HA | 2 | 0.13 |
| (1,2492) | 1:77:A:LEU:HD12 | 1:86:A:TYR:HA | 2 | 0.13 |
| (1,2492) | 1:77:A:LEU:HD13 | 1:86:A:TYR:HA | 2 | 0.13 |
| (1,2492) | 1:77:A:LEU:HD21 | 1:86:A:TYR:HA | 2 | 0.13 |
| (1,2492) | 1:77:A:LEU:HD22 | 1:86:A:TYR:HA | 2 | 0.13 |
| (1,2492) | 1:77:A:LEU:HD23 | 1:86:A:TYR:HA | 2 | 0.13 |
| (1,2486) | 1:43:A:ILE:HD11 | 1:86:A:TYR:HB2 | 20 | 0.13 |
| (1,2486) | 1:43:A:ILE:HD11 | 1:86:A:TYR:HB3 | 20 | 0.13 |
| (1,2486) | 1:43:A:ILE:HD12 | 1:86:A:TYR:HB2 | 20 | 0.13 |
| (1,2486) | 1:43:A:ILE:HD12 | 1:86:A:TYR:HB3 | 20 | 0.13 |
| (1,2486) | 1:43:A:ILE:HD13 | 1:86:A:TYR:HB2 | 20 | 0.13 |
| (1,2486) | 1:43:A:ILE:HD13 | 1:86:A:TYR:HB3 | 20 | 0.13 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 11 | 0.13 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 11 | 0.13 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 20 | 0.13 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 20 | 0.13 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 11 | 0.13 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 11 | 0.13 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 20 | 0.13 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 20 | 0.13 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 11 | 0.13 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 11 | 0.13 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 20 | 0.13 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 20 | 0.13 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB2 | 14 | 0.13 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB3 | 14 | 0.13 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB2 | 17 | 0.13 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB3 | 17 | 0.13 |
| (1,2308) | 1:67:A:ALA:HB1 | 1:68:A:ARG:HE | 4 | 0.13 |
| (1,2308) | 1:67:A:ALA:HB2 | 1:68:A:ARG:HE | 4 | 0.13 |
| (1,2308) | 1:67:A:ALA:HB3 | 1:68:A:ARG:HE | 4 | 0.13 |
| (1,2241) | 1:58:A:THR:HG21 | 1:61:A:VAL:HB | 14 | 0.13 |
| (1,2241) | 1:58:A:THR:HG22 | 1:61:A:VAL:HB | 14 | 0.13 |
| (1,2241) | 1:58:A:THR:HG23 | 1:61:A:VAL:HB | 14 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG21 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG22 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG23 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG21 | 17 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG22 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG23 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG21 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG22 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG23 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG21 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG22 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG23 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG21 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG22 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG23 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG21 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG22 | 17 | 0.13 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG23 | 17 | 0.13 |
| (1,2217) | 1:56:A:ALA:HB1 | 1:58:A:THR:HB | 15 | 0.13 |
| (1,2217) | 1:56:A:ALA:HB2 | 1:58:A:THR:HB | 15 | 0.13 |
| (1,2217) | 1:56:A:ALA:HB3 | 1:58:A:THR:HB | 15 | 0.13 |
| (1,2163) | 1:50:A:ARG:HD2 | 1:52:A:ALA:HA | 17 | 0.13 |
| (1,2163) | 1:50:A:ARG:HD3 | 1:52:A:ALA:HA | 17 | 0.13 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 5 | 0.13 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 5 | 0.13 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 6 | 0.13 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 6 | 0.13 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB2 | 17 | 0.13 |
| (1,2116) | 1:45:A:SER:H | 1:46:A:SER:HB3 | 17 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 17 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 17 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 17 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 17 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 17 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 17 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 20 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 20 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 20 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 20 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 20 | 0.13 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 20 | 0.13 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG21 | 3 | 0.13 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG22 | 3 | 0.13 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG23 | 3 | 0.13 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG21 | 3 | 0.13 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG22 | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG23 | 3 | 0.13 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD11 | 5 | 0.13 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD12 | 5 | 0.13 |
| (1,2084) | 1:41:A:GLN:HB2 | 1:43:A:ILE:HD13 | 5 | 0.13 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD11 | 5 | 0.13 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD12 | 5 | 0.13 |
| (1,2084) | 1:41:A:GLN:HB3 | 1:43:A:ILE:HD13 | 5 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG11 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG12 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG13 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG21 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG22 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD2 | 1:39:A:VAL:HG23 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG11 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG12 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG13 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG21 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG22 | 9 | 0.13 |
| (1,2034) | 1:36:A:ARG:HD3 | 1:39:A:VAL:HG23 | 9 | 0.13 |
| (1,1989) | 1:33:A:THR:HB | 1:34:A:VAL:H | 10 | 0.13 |
| (1,1962) | 1:19:A:SER:HA | 1:31:A:LEU:HB2 | 17 | 0.13 |
| (1,1962) | 1:19:A:SER:HA | 1:31:A:LEU:HB3 | 17 | 0.13 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD11 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD12 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD13 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD21 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD22 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG21 | 1:31:A:LEU:HD23 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD11 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD12 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD13 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD21 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD22 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG22 | 1:31:A:LEU:HD23 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD11 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD12 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD13 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD21 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD22 | 8 | 0.13 |
| (1,1956) | 1:30:A:THR:HG23 | 1:31:A:LEU:HD23 | 8 | 0.13 |
| (1,1904) | 1:20:A:ARG:HA | 1:24:A:ALA:HA | 4 | 0.13 |
| (1,1904) | 1:20:A:ARG:HA | 1:24:A:ALA:HA | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG11 | 8 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG12 | 8 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG13 | 8 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG21 | 8 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG22 | 8 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG23 | 8 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG11 | 15 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG12 | 15 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG13 | 15 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG21 | 15 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG22 | 15 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG23 | 15 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG11 | 17 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG12 | 17 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG13 | 17 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG21 | 17 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG22 | 17 | 0.13 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG23 | 17 | 0.13 |
| (1,1777) | 1:153:A:SER:H | 1:153:A:SER:HA | 2 | 0.13 |
| (1,1777) | 1:153:A:SER:H | 1:153:A:SER:HA | 14 | 0.13 |
| (1,1697) | 1:144:A:SER:H | 1:146:A:PHE:HB2 | 10 | 0.13 |
| (1,1697) | 1:144:A:SER:H | 1:146:A:PHE:HB3 | 10 | 0.13 |
| (1,1660) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 5 | 0.13 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 10 | 0.13 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 11 | 0.13 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 12 | 0.13 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 15 | 0.13 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 2 | 0.13 |
| (1,1483) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 8 | 0.13 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD11 | 19 | 0.13 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD12 | 19 | 0.13 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD13 | 19 | 0.13 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD21 | 19 | 0.13 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD22 | 19 | 0.13 |
| (1,1429) | 1:62:A:ASP:H | 1:66:A:LEU:HD23 | 19 | 0.13 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD2 | 3 | 0.13 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 3 | 0.13 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD2 | 8 | 0.13 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 8 | 0.13 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 5 | 0.13 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 5 | 0.13 |
| (1,1281) | 1:33:A:THR:HB | 1:34:A:VAL:H | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|------------------|----------|---------------|
| (1,1257) | 1:27:A:ASN:H | 1:27:A:ASN:HB2 | 4 | 0.13 |
| (1,1257) | 1:27:A:ASN:H | 1:27:A:ASN:HB3 | 4 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG11 | 3 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG12 | 3 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG13 | 3 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG21 | 3 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG22 | 3 | 0.13 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG23 | 3 | 0.13 |
| (1,1156) | 1:34:A:VAL:H | 1:34:A:VAL:HA | 10 | 0.13 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 3 | 0.13 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 5 | 0.13 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 9 | 0.13 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 12 | 0.13 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 13 | 0.13 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 15 | 0.13 |
| (1,1127) | 1:163:A:SER:H | 1:162:A:SER:HA | 5 | 0.13 |
| (1,1123) | 1:132:A:ASP:H | 1:136:A:VAL:HB | 5 | 0.13 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG11 | 13 | 0.13 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG12 | 13 | 0.13 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG13 | 13 | 0.13 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG21 | 13 | 0.13 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG22 | 13 | 0.13 |
| (1,1114) | 1:69:A:PHE:H | 1:71:A:VAL:HG23 | 13 | 0.13 |
| (1,1107) | 1:109:A:GLY:H | 1:112:A:VAL:HB | 4 | 0.13 |
| (1,1107) | 1:109:A:GLY:H | 1:112:A:VAL:HB | 8 | 0.13 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD11 | 20 | 0.13 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD12 | 20 | 0.13 |
| (1,1077) | 1:92:A:SER:H | 1:18:A:ILE:HD13 | 20 | 0.13 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 16 | 0.13 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 11 | 0.13 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 11 | 0.13 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 11 | 0.13 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 11 | 0.13 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 11 | 0.13 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 11 | 0.13 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 8 | 0.13 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 8 | 0.13 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD11 | 5 | 0.13 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD12 | 5 | 0.13 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD13 | 5 | 0.13 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD21 | 5 | 0.13 |
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD22 | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,988) | 1:23:A:ASN:H | 1:31:A:LEU:HD23 | 5 | 0.13 |
| (1,975) | 1:60:A:GLY:HA2 | 1:62:A:ASP:H | 3 | 0.13 |
| (1,975) | 1:60:A:GLY:HA3 | 1:62:A:ASP:H | 3 | 0.13 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 18 | 0.13 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 18 | 0.13 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 18 | 0.13 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB2 | 7 | 0.13 |
| (1,942) | 1:194:A:GLN:H | 1:194:A:GLN:HB3 | 7 | 0.13 |
| (1,940) | 1:191:A:PRO:HD2 | 1:193:A:GLY:H | 8 | 0.13 |
| (1,940) | 1:191:A:PRO:HD3 | 1:193:A:GLY:H | 8 | 0.13 |
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 14 | 0.13 |
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 14 | 0.13 |
| (1,932) | 1:190:A:ALA:H | 1:191:A:PRO:HD2 | 19 | 0.13 |
| (1,932) | 1:190:A:ALA:H | 1:191:A:PRO:HD3 | 19 | 0.13 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 6 | 0.13 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG2 | 17 | 0.13 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG3 | 17 | 0.13 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB2 | 12 | 0.13 |
| (1,901) | 1:163:A:SER:H | 1:163:A:SER:HB3 | 12 | 0.13 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB2 | 5 | 0.13 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB3 | 5 | 0.13 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB2 | 20 | 0.13 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB3 | 20 | 0.13 |
| (1,875) | 1:148:A:SER:HB2 | 1:149:A:THR:H | 15 | 0.13 |
| (1,875) | 1:148:A:SER:HB3 | 1:149:A:THR:H | 15 | 0.13 |
| (1,870) | 1:27:A:ASN:HB2 | 1:147:A:LEU:H | 15 | 0.13 |
| (1,870) | 1:27:A:ASN:HB3 | 1:147:A:LEU:H | 15 | 0.13 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 12 | 0.13 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 12 | 0.13 |
| (1,826) | 1:131:A:VAL:HB | 1:136:A:VAL:H | 9 | 0.13 |
| (1,824) | 1:37:A:THR:HG21 | 1:136:A:VAL:H | 6 | 0.13 |
| (1,824) | 1:37:A:THR:HG22 | 1:136:A:VAL:H | 6 | 0.13 |
| (1,824) | 1:37:A:THR:HG23 | 1:136:A:VAL:H | 6 | 0.13 |
| (1,815) | 1:132:A:ASP:HB2 | 1:135:A:SER:H | 17 | 0.13 |
| (1,815) | 1:132:A:ASP:HB3 | 1:135:A:SER:H | 17 | 0.13 |
| (1,801) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 5 | 0.13 |
| (1,781) | 1:127:A:LEU:H | 1:129:A:ILE:H | 13 | 0.13 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA2 | 5 | 0.13 |
| (1,771) | 1:127:A:LEU:H | 1:128:A:GLY:HA3 | 5 | 0.13 |
| (1,728) | 1:116:A:LEU:H | 1:120:A:VAL:H | 15 | 0.13 |
| (1,670) | 1:10:A:THR:H | 1:113:A:LEU:HD11 | 10 | 0.13 |
| (1,670) | 1:10:A:THR:H | 1:113:A:LEU:HD12 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,670) | 1:10:A:THR:H | 1:113:A:LEU:HD13 | 10 | 0.13 |
| (1,670) | 1:10:A:THR:H | 1:113:A:LEU:HD21 | 10 | 0.13 |
| (1,670) | 1:10:A:THR:H | 1:113:A:LEU:HD22 | 10 | 0.13 |
| (1,670) | 1:10:A:THR:H | 1:113:A:LEU:HD23 | 10 | 0.13 |
| (1,633) | 1:14:A:SER:H | 1:108:A:LEU:HB2 | 2 | 0.13 |
| (1,633) | 1:14:A:SER:H | 1:108:A:LEU:HB3 | 2 | 0.13 |
| (1,455) | 1:83:A:THR:HG21 | 1:84:A:SER:H | 11 | 0.13 |
| (1,455) | 1:83:A:THR:HG22 | 1:84:A:SER:H | 11 | 0.13 |
| (1,455) | 1:83:A:THR:HG23 | 1:84:A:SER:H | 11 | 0.13 |
| (1,433) | 1:79:A:ALA:HA | 1:80:A:GLY:H | 8 | 0.13 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG11 | 5 | 0.13 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG12 | 5 | 0.13 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG13 | 5 | 0.13 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG21 | 5 | 0.13 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG22 | 5 | 0.13 |
| (1,405) | 1:47:A:VAL:H | 1:74:A:VAL:HG23 | 5 | 0.13 |
| (1,362) | 1:66:A:LEU:HG | 1:68:A:ARG:H | 10 | 0.13 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD21 | 13 | 0.13 |
| (1,342) | 1:60:A:GLY:HA2 | 1:65:A:ASN:HD22 | 13 | 0.13 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD21 | 13 | 0.13 |
| (1,342) | 1:60:A:GLY:HA3 | 1:65:A:ASN:HD22 | 13 | 0.13 |
| (1,295) | 1:50:A:ARG:HB2 | 1:57:A:SER:H | 17 | 0.13 |
| (1,295) | 1:50:A:ARG:HB3 | 1:57:A:SER:H | 17 | 0.13 |
| (1,268) | 1:50:A:ARG:HG2 | 1:53:A:GLN:H | 17 | 0.13 |
| (1,268) | 1:50:A:ARG:HG3 | 1:53:A:GLN:H | 17 | 0.13 |
| (1,257) | 1:50:A:ARG:H | 1:51:A:ALA:H | 10 | 0.13 |
| (1,256) | 1:50:A:ARG:H | 1:51:A:ALA:H | 10 | 0.13 |
| (1,231) | 1:46:A:SER:H | 1:47:A:VAL:H | 19 | 0.13 |
| (1,230) | 1:46:A:SER:H | 1:47:A:VAL:H | 19 | 0.13 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 13 | 0.13 |
| (1,101) | 1:27:A:ASN:H | 1:27:A:ASN:HB2 | 4 | 0.13 |
| (1,101) | 1:27:A:ASN:H | 1:27:A:ASN:HB3 | 4 | 0.13 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 3 | 0.12 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 4 | 0.12 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 10 | 0.12 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 14 | 0.12 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD11 | 7 | 0.12 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD12 | 7 | 0.12 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD13 | 7 | 0.12 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD21 | 7 | 0.12 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD22 | 7 | 0.12 |
| (1,3863) | 1:129:A:ILE:HG13 | 1:55:A:LEU:HD23 | 7 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3858) | 1:110:A:SER:H | 1:111:A:ARG:HG2 | 7 | 0.12 |
| (1,3858) | 1:110:A:SER:H | 1:111:A:ARG:HG3 | 7 | 0.12 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB2 | 5 | 0.12 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB3 | 5 | 0.12 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB2 | 16 | 0.12 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB3 | 16 | 0.12 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB2 | 13 | 0.12 |
| (1,3760) | 1:85:A:ALA:HA | 1:82:A:ASP:HB3 | 13 | 0.12 |
| (1,3735) | 1:48:A:VAL:HG23 | 1:46:A:SER:H | 9 | 0.12 |
| (1,3711) | 1:149:A:THR:H | 1:149:A:THR:HA | 7 | 0.12 |
| (1,3711) | 1:149:A:THR:H | 1:149:A:THR:HA | 12 | 0.12 |
| (1,3711) | 1:149:A:THR:H | 1:149:A:THR:HA | 17 | 0.12 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB2 | 5 | 0.12 |
| (1,3697) | 1:13:A:ALA:HB3 | 1:108:A:LEU:HB3 | 5 | 0.12 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB2 | 10 | 0.12 |
| (1,3696) | 1:129:A:ILE:HG23 | 1:50:A:ARG:HB3 | 10 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB1 | 1:87:A:ALA:HB1 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB1 | 1:87:A:ALA:HB2 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB1 | 1:87:A:ALA:HB3 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB2 | 1:87:A:ALA:HB1 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB2 | 1:87:A:ALA:HB2 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB2 | 1:87:A:ALA:HB3 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB3 | 1:87:A:ALA:HB1 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB3 | 1:87:A:ALA:HB2 | 16 | 0.12 |
| (1,3687) | 1:89:A:ALA:HB3 | 1:87:A:ALA:HB3 | 16 | 0.12 |
| (1,3683) | 1:56:A:ALA:HB3 | 1:50:A:ARG:HA | 2 | 0.12 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB2 | 17 | 0.12 |
| (1,3672) | 1:32:A:ARG:HA | 1:88:A:GLN:HB3 | 17 | 0.12 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG21 | 11 | 0.12 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG22 | 11 | 0.12 |
| (1,3665) | 1:19:A:SER:HB2 | 1:18:A:ILE:HG23 | 11 | 0.12 |
| (1,3649) | 1:129:A:ILE:HG21 | 1:131:A:VAL:H | 9 | 0.12 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE1 | 12 | 0.12 |
| (1,3623) | 1:140:A:ILE:HD12 | 1:95:A:PHE:HE2 | 12 | 0.12 |
| (1,3622) | 1:122:A:SER:H | 1:55:A:LEU:HD11 | 15 | 0.12 |
| (1,3622) | 1:122:A:SER:H | 1:55:A:LEU:HD12 | 15 | 0.12 |
| (1,3622) | 1:122:A:SER:H | 1:55:A:LEU:HD13 | 15 | 0.12 |
| (1,3622) | 1:122:A:SER:H | 1:55:A:LEU:HD21 | 15 | 0.12 |
| (1,3622) | 1:122:A:SER:H | 1:55:A:LEU:HD22 | 15 | 0.12 |
| (1,3622) | 1:122:A:SER:H | 1:55:A:LEU:HD23 | 15 | 0.12 |
| (1,3617) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HB2 | 19 | 0.12 |
| (1,3617) | 1:124:A:ALA:HB2 | 1:125:A:GLN:HB3 | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD11 | 10 | 0.12 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD12 | 10 | 0.12 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD13 | 10 | 0.12 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD21 | 10 | 0.12 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD22 | 10 | 0.12 |
| (1,3602) | 1:95:A:PHE:HA | 1:94:A:LEU:HD23 | 10 | 0.12 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG11 | 9 | 0.12 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG12 | 9 | 0.12 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG13 | 9 | 0.12 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG21 | 9 | 0.12 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG22 | 9 | 0.12 |
| (1,3599) | 1:129:A:ILE:HG22 | 1:39:A:VAL:HG23 | 9 | 0.12 |
| (1,3559) | 1:156:A:TYR:HA | 1:155:A:SER:HB2 | 14 | 0.12 |
| (1,3559) | 1:156:A:TYR:HA | 1:155:A:SER:HB3 | 14 | 0.12 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG2 | 8 | 0.12 |
| (1,3520) | 1:129:A:ILE:HG13 | 1:50:A:ARG:HG3 | 8 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 3 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 3 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 3 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 3 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 18 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 18 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 18 | 0.12 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 18 | 0.12 |
| (1,3515) | 1:31:A:LEU:HD22 | 1:31:A:LEU:HA | 4 | 0.12 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD11 | 19 | 0.12 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD12 | 19 | 0.12 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD13 | 19 | 0.12 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD21 | 19 | 0.12 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD22 | 19 | 0.12 |
| (1,3479) | 1:121:A:SER:HA | 1:117:A:LEU:HD23 | 19 | 0.12 |
| (1,3466) | 1:7:A:PHE:HA | 1:6:A:GLY:HA2 | 15 | 0.12 |
| (1,3466) | 1:7:A:PHE:HA | 1:6:A:GLY:HA3 | 15 | 0.12 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB2 | 4 | 0.12 |
| (1,3423) | 1:9:A:ALA:H | 1:42:A:GLN:HB3 | 4 | 0.12 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:52:A:ALA:HB1 | 11 | 0.12 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:52:A:ALA:HB2 | 11 | 0.12 |
| (1,3372) | 1:53:A:GLN:HB3 | 1:52:A:ALA:HB3 | 11 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD11 | 1:105:A:ILE:HD11 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD11 | 1:105:A:ILE:HD12 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD11 | 1:105:A:ILE:HD13 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD12 | 1:105:A:ILE:HD11 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3364) | 1:108:A:LEU:HD12 | 1:105:A:ILE:HD12 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD12 | 1:105:A:ILE:HD13 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD13 | 1:105:A:ILE:HD11 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD13 | 1:105:A:ILE:HD12 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD13 | 1:105:A:ILE:HD13 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD21 | 1:105:A:ILE:HD11 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD21 | 1:105:A:ILE:HD12 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD21 | 1:105:A:ILE:HD13 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD22 | 1:105:A:ILE:HD11 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD22 | 1:105:A:ILE:HD12 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD22 | 1:105:A:ILE:HD13 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD23 | 1:105:A:ILE:HD11 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD23 | 1:105:A:ILE:HD12 | 15 | 0.12 |
| (1,3364) | 1:108:A:LEU:HD23 | 1:105:A:ILE:HD13 | 15 | 0.12 |
| (1,3351) | 1:7:A:PHE:HA | 1:6:A:GLY:HA2 | 15 | 0.12 |
| (1,3351) | 1:7:A:PHE:HA | 1:6:A:GLY:HA3 | 15 | 0.12 |
| (1,3334) | 1:188:A:GLY:HA2 | 1:190:A:ALA:HA | 19 | 0.12 |
| (1,3334) | 1:188:A:GLY:HA3 | 1:190:A:ALA:HA | 19 | 0.12 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 17 | 0.12 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 17 | 0.12 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 17 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB2 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD11 | 1:121:A:SER:HB3 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB2 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD12 | 1:121:A:SER:HB3 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB2 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD13 | 1:121:A:SER:HB3 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB2 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD21 | 1:121:A:SER:HB3 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB2 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD22 | 1:121:A:SER:HB3 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB2 | 4 | 0.12 |
| (1,3275) | 1:55:A:LEU:HD23 | 1:121:A:SER:HB3 | 4 | 0.12 |
| (1,3254) | 1:163:A:SER:H | 1:162:A:SER:HA | 1 | 0.12 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 10 | 0.12 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 10 | 0.12 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 10 | 0.12 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 10 | 0.12 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 10 | 0.12 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 10 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD11 | 1:194:A:GLN:HG2 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD11 | 1:194:A:GLN:HG3 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3201) | 1:186:A:LEU:HD12 | 1:194:A:GLN:HG2 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD12 | 1:194:A:GLN:HG3 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD13 | 1:194:A:GLN:HG2 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD13 | 1:194:A:GLN:HG3 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD21 | 1:194:A:GLN:HG2 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD21 | 1:194:A:GLN:HG3 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD22 | 1:194:A:GLN:HG2 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD22 | 1:194:A:GLN:HG3 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD23 | 1:194:A:GLN:HG2 | 6 | 0.12 |
| (1,3201) | 1:186:A:LEU:HD23 | 1:194:A:GLN:HG3 | 6 | 0.12 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB2 | 19 | 0.12 |
| (1,3198) | 1:190:A:ALA:HB1 | 1:194:A:GLN:HB3 | 19 | 0.12 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB2 | 19 | 0.12 |
| (1,3198) | 1:190:A:ALA:HB2 | 1:194:A:GLN:HB3 | 19 | 0.12 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB2 | 19 | 0.12 |
| (1,3198) | 1:190:A:ALA:HB3 | 1:194:A:GLN:HB3 | 19 | 0.12 |
| (1,3185) | 1:20:A:ARG:HD2 | 1:191:A:PRO:HA | 19 | 0.12 |
| (1,3185) | 1:20:A:ARG:HD3 | 1:191:A:PRO:HA | 19 | 0.12 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD2 | 6 | 0.12 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD3 | 6 | 0.12 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD2 | 9 | 0.12 |
| (1,3184) | 1:20:A:ARG:HA | 1:191:A:PRO:HD3 | 9 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA2 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD11 | 1:178:A:GLY:HA3 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA2 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD12 | 1:178:A:GLY:HA3 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA2 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD13 | 1:178:A:GLY:HA3 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA2 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD21 | 1:178:A:GLY:HA3 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA2 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD22 | 1:178:A:GLY:HA3 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA2 | 15 | 0.12 |
| (1,3146) | 1:25:A:LEU:HD23 | 1:178:A:GLY:HA3 | 15 | 0.12 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG21 | 2 | 0.12 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG22 | 2 | 0.12 |
| (1,3145) | 1:170:A:THR:HB | 1:177:A:THR:HG23 | 2 | 0.12 |
| (1,3108) | 1:153:A:SER:HA | 1:158:A:GLN:HB2 | 10 | 0.12 |
| (1,3108) | 1:153:A:SER:HA | 1:158:A:GLN:HB3 | 10 | 0.12 |
| (1,3021) | 1:28:A:THR:HG21 | 1:139:A:ASP:HA | 17 | 0.12 |
| (1,3021) | 1:28:A:THR:HG22 | 1:139:A:ASP:HA | 17 | 0.12 |
| (1,3021) | 1:28:A:THR:HG23 | 1:139:A:ASP:HA | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2891) | 1:36:A:ARG:HE | 1:124:A:ALA:HB1 | 18 | 0.12 |
| (1,2891) | 1:36:A:ARG:HE | 1:124:A:ALA:HB2 | 18 | 0.12 |
| (1,2891) | 1:36:A:ARG:HE | 1:124:A:ALA:HB3 | 18 | 0.12 |
| (1,2846) | 1:117:A:LEU:HG | 1:118:A:ASN:HD21 | 18 | 0.12 |
| (1,2846) | 1:117:A:LEU:HG | 1:118:A:ASN:HD22 | 18 | 0.12 |
| (1,2839) | 1:105:A:ILE:HG12 | 1:117:A:LEU:HB2 | 20 | 0.12 |
| (1,2839) | 1:105:A:ILE:HG12 | 1:117:A:LEU:HB3 | 20 | 0.12 |
| (1,2839) | 1:105:A:ILE:HG13 | 1:117:A:LEU:HB2 | 20 | 0.12 |
| (1,2839) | 1:105:A:ILE:HG13 | 1:117:A:LEU:HB3 | 20 | 0.12 |
| (1,2838) | 1:94:A:LEU:HA | 1:117:A:LEU:HD11 | 13 | 0.12 |
| (1,2838) | 1:94:A:LEU:HA | 1:117:A:LEU:HD12 | 13 | 0.12 |
| (1,2838) | 1:94:A:LEU:HA | 1:117:A:LEU:HD13 | 13 | 0.12 |
| (1,2838) | 1:94:A:LEU:HA | 1:117:A:LEU:HD21 | 13 | 0.12 |
| (1,2838) | 1:94:A:LEU:HA | 1:117:A:LEU:HD22 | 13 | 0.12 |
| (1,2838) | 1:94:A:LEU:HA | 1:117:A:LEU:HD23 | 13 | 0.12 |
| (1,2731) | 1:108:A:LEU:HG | 1:109:A:GLY:HA2 | 19 | 0.12 |
| (1,2731) | 1:108:A:LEU:HG | 1:109:A:GLY:HA3 | 19 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD11 | 11 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD12 | 11 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD13 | 11 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD21 | 11 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD22 | 11 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD23 | 11 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD11 | 17 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD12 | 17 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD13 | 17 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD21 | 17 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD22 | 17 | 0.12 |
| (1,2727) | 1:10:A:THR:HA | 1:108:A:LEU:HD23 | 17 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 15 | 0.12 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 15 | 0.12 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 5 | 0.12 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 5 | 0.12 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 5 | 0.12 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 5 | 0.12 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 5 | 0.12 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 5 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 16 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 16 | 0.12 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 16 | 0.12 |
| (1,2644) | 1:96:A:ASN:HB2 | 1:100:A:LEU:HG | 11 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,2644) | 1:96:A:ASN:HB3 | 1:100:A:LEU:HG | 11 | 0.12 |
| (1,2641) | 1:97:A:ALA:HB1 | 1:100:A:LEU:HG | 17 | 0.12 |
| (1,2641) | 1:97:A:ALA:HB2 | 1:100:A:LEU:HG | 17 | 0.12 |
| (1,2641) | 1:97:A:ALA:HB3 | 1:100:A:LEU:HG | 17 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD11 | 6 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD12 | 6 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD13 | 6 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD21 | 6 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD22 | 6 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD23 | 6 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD11 | 11 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD12 | 11 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD13 | 11 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD21 | 11 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD22 | 11 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD23 | 11 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD11 | 19 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD12 | 19 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD13 | 19 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD21 | 19 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD22 | 19 | 0.12 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD23 | 19 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 4 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 4 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 4 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 4 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 4 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 4 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 8 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 8 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 8 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 8 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 8 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 8 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 18 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 18 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 18 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 18 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 18 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 18 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 19 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 19 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 19 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 19 | 0.12 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 19 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG11 | 1:93:A:ALA:HA | 6 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG12 | 1:93:A:ALA:HA | 6 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG13 | 1:93:A:ALA:HA | 6 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG21 | 1:93:A:ALA:HA | 6 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG22 | 1:93:A:ALA:HA | 6 | 0.12 |
| (1,2558) | 1:21:A:VAL:HG23 | 1:93:A:ALA:HA | 6 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG11 | 1:88:A:GLN:HE21 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG11 | 1:88:A:GLN:HE22 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG12 | 1:88:A:GLN:HE21 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG12 | 1:88:A:GLN:HE22 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG13 | 1:88:A:GLN:HE21 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG13 | 1:88:A:GLN:HE22 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG21 | 1:88:A:GLN:HE21 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG21 | 1:88:A:GLN:HE22 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG22 | 1:88:A:GLN:HE21 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG22 | 1:88:A:GLN:HE22 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG23 | 1:88:A:GLN:HE21 | 2 | 0.12 |
| (1,2521) | 1:34:A:VAL:HG23 | 1:88:A:GLN:HE22 | 2 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD11 | 1:86:A:TYR:HA | 5 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD12 | 1:86:A:TYR:HA | 5 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD13 | 1:86:A:TYR:HA | 5 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD21 | 1:86:A:TYR:HA | 5 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD22 | 1:86:A:TYR:HA | 5 | 0.12 |
| (1,2492) | 1:77:A:LEU:HD23 | 1:86:A:TYR:HA | 5 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE1 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE2 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE1 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE2 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE1 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE2 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE1 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE2 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE1 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE2 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE1 | 16 | 0.12 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE2 | 16 | 0.12 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG2 | 17 | 0.12 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG3 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2430) | 1:43:A:ILE:HD11 | 1:77:A:LEU:HG | 17 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 5 | 0.12 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 5 | 0.12 |
| (1,2328) | 1:48:A:VAL:HA | 1:70:A:ALA:HA | 10 | 0.12 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB2 | 9 | 0.12 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB3 | 9 | 0.12 |
| (1,2281) | 1:61:A:VAL:HB | 1:66:A:LEU:HB2 | 19 | 0.12 |
| (1,2281) | 1:61:A:VAL:HB | 1:66:A:LEU:HB3 | 19 | 0.12 |
| (1,2280) | 1:62:A:ASP:HA | 1:66:A:LEU:HG | 5 | 0.12 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD21 | 12 | 0.12 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD22 | 12 | 0.12 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD21 | 12 | 0.12 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD22 | 12 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG11 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG12 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG13 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG21 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG22 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG23 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG11 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG12 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG13 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG21 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG22 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG23 | 6 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG11 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG12 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG13 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG21 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG22 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB2 | 1:61:A:VAL:HG23 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG11 | 10 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG12 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG13 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG21 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG22 | 10 | 0.12 |
| (1,2244) | 1:53:A:GLN:HB3 | 1:61:A:VAL:HG23 | 10 | 0.12 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB2 | 12 | 0.12 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB3 | 12 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 6 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 6 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 10 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 10 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 18 | 0.12 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 18 | 0.12 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 10 | 0.12 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 10 | 0.12 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 10 | 0.12 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 10 | 0.12 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 10 | 0.12 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 10 | 0.12 |
| (1,2002) | 1:34:A:VAL:HB | 1:35:A:LEU:H | 19 | 0.12 |
| (1,1957) | 1:30:A:THR:HG21 | 1:31:A:LEU:H | 1 | 0.12 |
| (1,1957) | 1:30:A:THR:HG22 | 1:31:A:LEU:H | 1 | 0.12 |
| (1,1957) | 1:30:A:THR:HG23 | 1:31:A:LEU:H | 1 | 0.12 |
| (1,1833) | 1:13:A:ALA:HA | 1:16:A:GLY:HA2 | 11 | 0.12 |
| (1,1833) | 1:13:A:ALA:HA | 1:16:A:GLY:HA3 | 11 | 0.12 |
| (1,1826) | 1:3:A:PRO:HA | 1:8:A:GLY:HA2 | 6 | 0.12 |
| (1,1826) | 1:3:A:PRO:HA | 1:8:A:GLY:HA3 | 6 | 0.12 |
| (1,1825) | 1:3:A:PRO:HA | 1:8:A:GLY:HA2 | 6 | 0.12 |
| (1,1825) | 1:3:A:PRO:HA | 1:8:A:GLY:HA3 | 6 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB2 | 9 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB3 | 9 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB2 | 9 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB3 | 9 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB2 | 15 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG2 | 1:7:A:PHE:HB3 | 15 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB2 | 15 | 0.12 |
| (1,1824) | 1:4:A:GLN:HG3 | 1:7:A:PHE:HB3 | 15 | 0.12 |
| (1,1707) | 1:149:A:THR:H | 1:149:A:THR:HA | 7 | 0.12 |
| (1,1707) | 1:149:A:THR:H | 1:149:A:THR:HA | 12 | 0.12 |
| (1,1707) | 1:149:A:THR:H | 1:149:A:THR:HA | 17 | 0.12 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 5 | 0.12 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 17 | 0.12 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 12 | 0.12 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 13 | 0.12 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 6 | 0.12 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 6 | 0.12 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 10 | 0.12 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 10 | 0.12 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 18 | 0.12 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 18 | 0.12 |
| (1,1168) | 1:22:A:ALA:H | 1:99:A:VAL:HG11 | 10 | 0.12 |
| (1,1168) | 1:22:A:ALA:H | 1:99:A:VAL:HG12 | 10 | 0.12 |
| (1,1168) | 1:22:A:ALA:H | 1:99:A:VAL:HG13 | 10 | 0.12 |
| (1,1168) | 1:22:A:ALA:H | 1:99:A:VAL:HG21 | 10 | 0.12 |
| (1,1168) | 1:22:A:ALA:H | 1:99:A:VAL:HG22 | 10 | 0.12 |
| (1,1168) | 1:22:A:ALA:H | 1:99:A:VAL:HG23 | 10 | 0.12 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 9 | 0.12 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 9 | 0.12 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG11 | 4 | 0.12 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG12 | 4 | 0.12 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG13 | 4 | 0.12 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG21 | 4 | 0.12 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG22 | 4 | 0.12 |
| (1,1163) | 1:111:A:ARG:H | 1:112:A:VAL:HG23 | 4 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB1 | 5 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB2 | 5 | 0.12 |
| (1,1157) | 1:121:A:SER:H | 1:124:A:ALA:HB3 | 5 | 0.12 |
| (1,1156) | 1:31:A:LEU:H | 1:31:A:LEU:HA | 9 | 0.12 |
| (1,1156) | 1:34:A:VAL:H | 1:34:A:VAL:HA | 12 | 0.12 |
| (1,1156) | 1:34:A:VAL:H | 1:34:A:VAL:HA | 16 | 0.12 |
| (1,1138) | 1:76:A:ARG:HB3 | 1:74:A:VAL:H | 20 | 0.12 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG21 | 8 | 0.12 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG22 | 8 | 0.12 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG23 | 8 | 0.12 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 4 | 0.12 |
| (1,1132) | 1:59:A:LEU:H | 1:59:A:LEU:HA | 10 | 0.12 |
| (1,1127) | 1:163:A:SER:H | 1:162:A:SER:HA | 1 | 0.12 |
| (1,1095) | 1:193:A:GLY:H | 1:191:A:PRO:HA | 15 | 0.12 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 17 | 0.12 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 19 | 0.12 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD11 | 17 | 0.12 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD12 | 17 | 0.12 |
| (1,1084) | 1:105:A:ILE:H | 1:105:A:ILE:HD13 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1073) | 1:61:A:VAL:HB | 1:62:A:ASP:H | 3 | 0.12 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 17 | 0.12 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 17 | 0.12 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 17 | 0.12 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB1 | 18 | 0.12 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB2 | 18 | 0.12 |
| (1,1063) | 1:126:A:GLY:H | 1:124:A:ALA:HB3 | 18 | 0.12 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 2 | 0.12 |
| (1,1023) | 1:164:A:THR:HA | 1:166:A:GLY:H | 8 | 0.12 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB2 | 20 | 0.12 |
| (1,1007) | 1:140:A:ILE:H | 1:137:A:GLN:HB3 | 20 | 0.12 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD11 | 6 | 0.12 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD12 | 6 | 0.12 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD13 | 6 | 0.12 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD21 | 6 | 0.12 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD22 | 6 | 0.12 |
| (1,974) | 1:26:A:ALA:H | 1:31:A:LEU:HD23 | 6 | 0.12 |
| (1,958) | 1:136:A:VAL:H | 1:140:A:ILE:H | 14 | 0.12 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 13 | 0.12 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 13 | 0.12 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 13 | 0.12 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG21 | 19 | 0.12 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG22 | 19 | 0.12 |
| (1,949) | 1:139:A:ASP:H | 1:140:A:ILE:HG23 | 19 | 0.12 |
| (1,946) | 1:196:A:GLY:H | 1:197:A:PHE:HA | 20 | 0.12 |
| (1,940) | 1:191:A:PRO:HD2 | 1:193:A:GLY:H | 17 | 0.12 |
| (1,940) | 1:191:A:PRO:HD3 | 1:193:A:GLY:H | 17 | 0.12 |
| (1,920) | 1:149:A:THR:HB | 1:180:A:SER:H | 16 | 0.12 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD2 | 5 | 0.12 |
| (1,914) | 1:170:A:THR:H | 1:175:A:PRO:HD3 | 5 | 0.12 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG2 | 14 | 0.12 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG3 | 14 | 0.12 |
| (1,897) | 1:156:A:TYR:HA | 1:160:A:SER:H | 4 | 0.12 |
| (1,897) | 1:156:A:TYR:HA | 1:160:A:SER:H | 7 | 0.12 |
| (1,893) | 1:153:A:SER:HB2 | 1:158:A:GLN:H | 13 | 0.12 |
| (1,893) | 1:153:A:SER:HB3 | 1:158:A:GLN:H | 13 | 0.12 |
| (1,876) | 1:148:A:SER:H | 1:149:A:THR:H | 1 | 0.12 |
| (1,876) | 1:148:A:SER:H | 1:149:A:THR:H | 2 | 0.12 |
| (1,857) | 1:140:A:ILE:H | 1:143:A:SER:HB2 | 2 | 0.12 |
| (1,857) | 1:140:A:ILE:H | 1:143:A:SER:HB3 | 2 | 0.12 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 3 | 0.12 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,648) | 1:108:A:LEU:HD11 | 1:110:A:SER:H | 20 | 0.12 |
| (1,648) | 1:108:A:LEU:HD12 | 1:110:A:SER:H | 20 | 0.12 |
| (1,648) | 1:108:A:LEU:HD13 | 1:110:A:SER:H | 20 | 0.12 |
| (1,648) | 1:108:A:LEU:HD21 | 1:110:A:SER:H | 20 | 0.12 |
| (1,648) | 1:108:A:LEU:HD22 | 1:110:A:SER:H | 20 | 0.12 |
| (1,648) | 1:108:A:LEU:HD23 | 1:110:A:SER:H | 20 | 0.12 |
| (1,631) | 1:104:A:ASN:H | 1:108:A:LEU:H | 20 | 0.12 |
| (1,595) | 1:100:A:LEU:HA | 1:104:A:ASN:HD21 | 4 | 0.12 |
| (1,595) | 1:100:A:LEU:HA | 1:104:A:ASN:HD22 | 4 | 0.12 |
| (1,594) | 1:100:A:LEU:HD11 | 1:104:A:ASN:H | 18 | 0.12 |
| (1,594) | 1:100:A:LEU:HD12 | 1:104:A:ASN:H | 18 | 0.12 |
| (1,594) | 1:100:A:LEU:HD13 | 1:104:A:ASN:H | 18 | 0.12 |
| (1,594) | 1:100:A:LEU:HD21 | 1:104:A:ASN:H | 18 | 0.12 |
| (1,594) | 1:100:A:LEU:HD22 | 1:104:A:ASN:H | 18 | 0.12 |
| (1,594) | 1:100:A:LEU:HD23 | 1:104:A:ASN:H | 18 | 0.12 |
| (1,589) | 1:101:A:ASN:H | 1:104:A:ASN:H | 1 | 0.12 |
| (1,589) | 1:101:A:ASN:H | 1:104:A:ASN:H | 3 | 0.12 |
| (1,589) | 1:101:A:ASN:H | 1:104:A:ASN:H | 13 | 0.12 |
| (1,561) | 1:22:A:ALA:H | 1:100:A:LEU:HA | 12 | 0.12 |
| (1,555) | 1:99:A:VAL:H | 1:100:A:LEU:HG | 13 | 0.12 |
| (1,483) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HE21 | 10 | 0.12 |
| (1,483) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HE22 | 10 | 0.12 |
| (1,483) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HE21 | 10 | 0.12 |
| (1,483) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HE22 | 10 | 0.12 |
| (1,482) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HE21 | 10 | 0.12 |
| (1,482) | 1:35:A:LEU:HB2 | 1:88:A:GLN:HE22 | 10 | 0.12 |
| (1,482) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HE21 | 10 | 0.12 |
| (1,482) | 1:35:A:LEU:HB3 | 1:88:A:GLN:HE22 | 10 | 0.12 |
| (1,339) | 1:63:A:GLY:H | 1:65:A:ASN:H | 19 | 0.12 |
| (1,332) | 1:61:A:VAL:HA | 1:64:A:ASN:H | 1 | 0.12 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 13 | 0.12 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG11 | 9 | 0.12 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG12 | 9 | 0.12 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG13 | 9 | 0.12 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG21 | 9 | 0.12 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG22 | 9 | 0.12 |
| (1,314) | 1:48:A:VAL:H | 1:61:A:VAL:HG23 | 9 | 0.12 |
| (1,268) | 1:50:A:ARG:HG2 | 1:53:A:GLN:H | 20 | 0.12 |
| (1,268) | 1:50:A:ARG:HG3 | 1:53:A:GLN:H | 20 | 0.12 |
| (1,258) | 1:49:A:GLN:HB2 | 1:51:A:ALA:H | 6 | 0.12 |
| (1,258) | 1:49:A:GLN:HB3 | 1:51:A:ALA:H | 6 | 0.12 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 10 | 0.12 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 19 | 0.12 |
| (1,69) | 1:21:A:VAL:HG11 | 1:22:A:ALA:H | 2 | 0.12 |
| (1,69) | 1:21:A:VAL:HG12 | 1:22:A:ALA:H | 2 | 0.12 |
| (1,69) | 1:21:A:VAL:HG13 | 1:22:A:ALA:H | 2 | 0.12 |
| (1,69) | 1:21:A:VAL:HG21 | 1:22:A:ALA:H | 2 | 0.12 |
| (1,69) | 1:21:A:VAL:HG22 | 1:22:A:ALA:H | 2 | 0.12 |
| (1,69) | 1:21:A:VAL:HG23 | 1:22:A:ALA:H | 2 | 0.12 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD1 | 11 | 0.11 |
| (1,3894) | 1:26:A:ALA:HB1 | 1:95:A:PHE:HD2 | 11 | 0.11 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD1 | 11 | 0.11 |
| (1,3894) | 1:26:A:ALA:HB2 | 1:95:A:PHE:HD2 | 11 | 0.11 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD1 | 11 | 0.11 |
| (1,3894) | 1:26:A:ALA:HB3 | 1:95:A:PHE:HD2 | 11 | 0.11 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 11 | 0.11 |
| (1,3866) | 1:177:A:THR:H | 1:177:A:THR:HA | 16 | 0.11 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB2 | 3 | 0.11 |
| (1,3807) | 1:141:A:SER:H | 1:143:A:SER:HB3 | 3 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB1 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB2 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG11 | 1:13:A:ALA:HB3 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB1 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB2 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG12 | 1:13:A:ALA:HB3 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB1 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB2 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG13 | 1:13:A:ALA:HB3 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB1 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB2 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG21 | 1:13:A:ALA:HB3 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB1 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB2 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG22 | 1:13:A:ALA:HB3 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB1 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB2 | 17 | 0.11 |
| (1,3761) | 1:112:A:VAL:HG23 | 1:13:A:ALA:HB3 | 17 | 0.11 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG21 | 4 | 0.11 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG22 | 4 | 0.11 |
| (1,3724) | 1:117:A:LEU:HB3 | 1:105:A:ILE:HG23 | 4 | 0.11 |
| (1,3711) | 1:149:A:THR:H | 1:149:A:THR:HA | 6 | 0.11 |
| (1,3711) | 1:149:A:THR:H | 1:149:A:THR:HA | 18 | 0.11 |
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB2 | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3697) | 1:13:A:ALA:HB2 | 1:108:A:LEU:HB3 | 4 | 0.11 |
| (1,3694) | 1:49:A:GLN:HA | 1:56:A:ALA:HB1 | 7 | 0.11 |
| (1,3694) | 1:49:A:GLN:HA | 1:56:A:ALA:HB2 | 7 | 0.11 |
| (1,3694) | 1:49:A:GLN:HA | 1:56:A:ALA:HB3 | 7 | 0.11 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD11 | 13 | 0.11 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD12 | 13 | 0.11 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD13 | 13 | 0.11 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD21 | 13 | 0.11 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD22 | 13 | 0.11 |
| (1,3660) | 1:185:A:PRO:HG2 | 1:186:A:LEU:HD23 | 13 | 0.11 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 14 | 0.11 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 14 | 0.11 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 14 | 0.11 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 14 | 0.11 |
| (1,3516) | 1:58:A:THR:HA | 1:59:A:LEU:HG | 17 | 0.11 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB2 | 6 | 0.11 |
| (1,3474) | 1:59:A:LEU:HB2 | 1:69:A:PHE:HB3 | 6 | 0.11 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB2 | 6 | 0.11 |
| (1,3474) | 1:59:A:LEU:HB3 | 1:69:A:PHE:HB3 | 6 | 0.11 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD11 | 12 | 0.11 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD12 | 12 | 0.11 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD13 | 12 | 0.11 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD21 | 12 | 0.11 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD22 | 12 | 0.11 |
| (1,3472) | 1:78:A:PRO:HG2 | 1:77:A:LEU:HD23 | 12 | 0.11 |
| (1,3471) | 1:76:A:ARG:HA | 1:72:A:GLN:HA | 2 | 0.11 |
| (1,3471) | 1:76:A:ARG:HA | 1:72:A:GLN:HA | 14 | 0.11 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 3 | 0.11 |
| (1,3423) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 3 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG2 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HG3 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG2 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HG3 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG2 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HG3 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG2 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HG3 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG2 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HG3 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG2 | 18 | 0.11 |
| (1,3419) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HG3 | 18 | 0.11 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 1 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 1 | 0.11 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 1 | 0.11 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 1 | 0.11 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 1 | 0.11 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 1 | 0.11 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD2 | 1 | 0.11 |
| (1,3381) | 1:177:A:THR:HG22 | 1:179:A:PRO:HD3 | 1 | 0.11 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD11 | 6 | 0.11 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD12 | 6 | 0.11 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD13 | 6 | 0.11 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD21 | 6 | 0.11 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD22 | 6 | 0.11 |
| (1,3325) | 1:126:A:GLY:H | 1:127:A:LEU:HD23 | 6 | 0.11 |
| (1,3279) | 1:178:A:GLY:HA2 | 1:177:A:THR:HB | 4 | 0.11 |
| (1,3279) | 1:178:A:GLY:HA3 | 1:177:A:THR:HB | 4 | 0.11 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 3 | 0.11 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 3 | 0.11 |
| (1,3278) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 3 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD11 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD12 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD13 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD21 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD22 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA2 | 1:100:A:LEU:HD23 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD11 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD12 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD13 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD21 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD22 | 10 | 0.11 |
| (1,3223) | 1:98:A:GLY:HA3 | 1:100:A:LEU:HD23 | 10 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 2 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 2 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 2 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 2 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 2 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 2 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 6 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 6 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 6 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 6 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 6 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 8 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 8 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 8 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 8 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 8 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 8 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 15 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 15 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 15 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 15 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 15 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 15 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 19 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 19 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 19 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 19 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 19 | 0.11 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 19 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB2 | 8 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB3 | 8 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB2 | 8 | 0.11 |
| (1,3207) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB3 | 8 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB2 | 8 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB3 | 8 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB2 | 8 | 0.11 |
| (1,3206) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB3 | 8 | 0.11 |
| (1,3204) | 1:101:A:ASN:H | 1:195:A:SER:HB2 | 15 | 0.11 |
| (1,3204) | 1:101:A:ASN:H | 1:195:A:SER:HB3 | 15 | 0.11 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG2 | 17 | 0.11 |
| (1,3203) | 1:186:A:LEU:HB2 | 1:194:A:GLN:HG3 | 17 | 0.11 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG2 | 17 | 0.11 |
| (1,3203) | 1:186:A:LEU:HB3 | 1:194:A:GLN:HG3 | 17 | 0.11 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 10 | 0.11 |
| (1,3186) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 10 | 0.11 |
| (1,3166) | 1:186:A:LEU:HD11 | 1:190:A:ALA:H | 1 | 0.11 |
| (1,3166) | 1:186:A:LEU:HD12 | 1:190:A:ALA:H | 1 | 0.11 |
| (1,3166) | 1:186:A:LEU:HD13 | 1:190:A:ALA:H | 1 | 0.11 |
| (1,3166) | 1:186:A:LEU:HD21 | 1:190:A:ALA:H | 1 | 0.11 |
| (1,3166) | 1:186:A:LEU:HD22 | 1:190:A:ALA:H | 1 | 0.11 |
| (1,3166) | 1:186:A:LEU:HD23 | 1:190:A:ALA:H | 1 | 0.11 |
| (1,3141) | 1:175:A:PRO:HD2 | 1:177:A:THR:HB | 18 | 0.11 |
| (1,3141) | 1:175:A:PRO:HD3 | 1:177:A:THR:HB | 18 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3122) | 1:20:A:ARG:HG2 | 1:171:A:GLY:HA2 | 3 | 0.11 |
| (1,3122) | 1:20:A:ARG:HG2 | 1:171:A:GLY:HA3 | 3 | 0.11 |
| (1,3122) | 1:20:A:ARG:HG3 | 1:171:A:GLY:HA2 | 3 | 0.11 |
| (1,3122) | 1:20:A:ARG:HG3 | 1:171:A:GLY:HA3 | 3 | 0.11 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB1 | 17 | 0.11 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB2 | 17 | 0.11 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB3 | 17 | 0.11 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG21 | 6 | 0.11 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG22 | 6 | 0.11 |
| (1,3089) | 1:27:A:ASN:HD21 | 1:149:A:THR:HG23 | 6 | 0.11 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG21 | 6 | 0.11 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG22 | 6 | 0.11 |
| (1,3089) | 1:27:A:ASN:HD22 | 1:149:A:THR:HG23 | 6 | 0.11 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB2 | 16 | 0.11 |
| (1,3067) | 1:28:A:THR:HB | 1:144:A:SER:HB3 | 16 | 0.11 |
| (1,3021) | 1:28:A:THR:HG21 | 1:139:A:ASP:HA | 4 | 0.11 |
| (1,3021) | 1:28:A:THR:HG22 | 1:139:A:ASP:HA | 4 | 0.11 |
| (1,3021) | 1:28:A:THR:HG23 | 1:139:A:ASP:HA | 4 | 0.11 |
| (1,2970) | 1:37:A:THR:HA | 1:131:A:VAL:HB | 19 | 0.11 |
| (1,2961) | 1:38:A:GLY:HA2 | 1:130:A:ASN:HA | 7 | 0.11 |
| (1,2961) | 1:38:A:GLY:HA3 | 1:130:A:ASN:HA | 7 | 0.11 |
| (1,2961) | 1:38:A:GLY:HA2 | 1:130:A:ASN:HA | 13 | 0.11 |
| (1,2961) | 1:38:A:GLY:HA3 | 1:130:A:ASN:HA | 13 | 0.11 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB2 | 16 | 0.11 |
| (1,2960) | 1:53:A:GLN:HE21 | 1:130:A:ASN:HB3 | 16 | 0.11 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB2 | 16 | 0.11 |
| (1,2960) | 1:53:A:GLN:HE22 | 1:130:A:ASN:HB3 | 16 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB2 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB3 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB2 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB3 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB2 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB3 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB2 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB3 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB2 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB3 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB2 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB3 | 13 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB2 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG11 | 1:125:A:GLN:HB3 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB2 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2908) | 1:120:A:VAL:HG12 | 1:125:A:GLN:HB3 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB2 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG13 | 1:125:A:GLN:HB3 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB2 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG21 | 1:125:A:GLN:HB3 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB2 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG22 | 1:125:A:GLN:HB3 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB2 | 15 | 0.11 |
| (1,2908) | 1:120:A:VAL:HG23 | 1:125:A:GLN:HB3 | 15 | 0.11 |
| (1,2906) | 1:105:A:ILE:HG21 | 1:125:A:GLN:HG2 | 15 | 0.11 |
| (1,2906) | 1:105:A:ILE:HG21 | 1:125:A:GLN:HG3 | 15 | 0.11 |
| (1,2906) | 1:105:A:ILE:HG22 | 1:125:A:GLN:HG2 | 15 | 0.11 |
| (1,2906) | 1:105:A:ILE:HG22 | 1:125:A:GLN:HG3 | 15 | 0.11 |
| (1,2906) | 1:105:A:ILE:HG23 | 1:125:A:GLN:HG2 | 15 | 0.11 |
| (1,2906) | 1:105:A:ILE:HG23 | 1:125:A:GLN:HG3 | 15 | 0.11 |
| (1,2880) | 1:120:A:VAL:HA | 1:123:A:ALA:HB1 | 5 | 0.11 |
| (1,2880) | 1:120:A:VAL:HA | 1:123:A:ALA:HB2 | 5 | 0.11 |
| (1,2880) | 1:120:A:VAL:HA | 1:123:A:ALA:HB3 | 5 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG11 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG12 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG13 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG21 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG22 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG2 | 1:120:A:VAL:HG23 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG11 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG12 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG13 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG21 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG22 | 8 | 0.11 |
| (1,2871) | 1:42:A:GLN:HG3 | 1:120:A:VAL:HG23 | 8 | 0.11 |
| (1,2851) | 1:115:A:ALA:HB1 | 1:118:A:ASN:HB2 | 15 | 0.11 |
| (1,2851) | 1:115:A:ALA:HB1 | 1:118:A:ASN:HB3 | 15 | 0.11 |
| (1,2851) | 1:115:A:ALA:HB2 | 1:118:A:ASN:HB2 | 15 | 0.11 |
| (1,2851) | 1:115:A:ALA:HB2 | 1:118:A:ASN:HB3 | 15 | 0.11 |
| (1,2851) | 1:115:A:ALA:HB3 | 1:118:A:ASN:HB2 | 15 | 0.11 |
| (1,2851) | 1:115:A:ALA:HB3 | 1:118:A:ASN:HB3 | 15 | 0.11 |
| (1,2835) | 1:110:A:SER:HA | 1:117:A:LEU:HA | 4 | 0.11 |
| (1,2835) | 1:110:A:SER:HA | 1:117:A:LEU:HA | 15 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD21 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2814) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2814) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD11 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD21 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2808) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD12 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD13 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD21 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD22 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD11 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD12 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD13 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD21 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD22 | 3 | 0.11 |
| (1,2808) | 1:55:A:LEU:HD23 | 1:116:A:LEU:HD23 | 3 | 0.11 |
| (1,2764) | 1:110:A:SER:HA | 1:112:A:VAL:H | 8 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB2 | 1:112:A:VAL:HG11 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB2 | 1:112:A:VAL:HG12 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB2 | 1:112:A:VAL:HG13 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB2 | 1:112:A:VAL:HG21 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB2 | 1:112:A:VAL:HG22 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB2 | 1:112:A:VAL:HG23 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB3 | 1:112:A:VAL:HG11 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB3 | 1:112:A:VAL:HG12 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB3 | 1:112:A:VAL:HG13 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB3 | 1:112:A:VAL:HG21 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB3 | 1:112:A:VAL:HG22 | 7 | 0.11 |
| (1,2761) | 1:111:A:ARG:HB3 | 1:112:A:VAL:HG23 | 7 | 0.11 |
| (1,2754) | 1:106:A:ASP:HA | 1:111:A:ARG:HD2 | 9 | 0.11 |
| (1,2754) | 1:106:A:ASP:HA | 1:111:A:ARG:HD3 | 9 | 0.11 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 13 | 0.11 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 13 | 0.11 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 13 | 0.11 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD2 | 18 | 0.11 |
| (1,2752) | 1:108:A:LEU:HB2 | 1:111:A:ARG:HD3 | 18 | 0.11 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD2 | 18 | 0.11 |
| (1,2752) | 1:108:A:LEU:HB3 | 1:111:A:ARG:HD3 | 18 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD11 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD12 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD13 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD21 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD22 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD11 | 1:108:A:LEU:HD23 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD11 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD12 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD13 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD21 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD22 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD12 | 1:108:A:LEU:HD23 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD11 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD12 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD13 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD21 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD22 | 14 | 0.11 |
| (1,2722) | 1:105:A:ILE:HD13 | 1:108:A:LEU:HD23 | 14 | 0.11 |
| (1,2720) | 1:107:A:THR:HG21 | 1:108:A:LEU:HB2 | 8 | 0.11 |
| (1,2720) | 1:107:A:THR:HG21 | 1:108:A:LEU:HB3 | 8 | 0.11 |
| (1,2720) | 1:107:A:THR:HG22 | 1:108:A:LEU:HB2 | 8 | 0.11 |
| (1,2720) | 1:107:A:THR:HG22 | 1:108:A:LEU:HB3 | 8 | 0.11 |
| (1,2720) | 1:107:A:THR:HG23 | 1:108:A:LEU:HB2 | 8 | 0.11 |
| (1,2720) | 1:107:A:THR:HG23 | 1:108:A:LEU:HB3 | 8 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 12 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 12 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 12 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 12 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 12 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 12 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG21 | 16 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG22 | 16 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB2 | 1:105:A:ILE:HG23 | 16 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG21 | 16 | 0.11 |
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG22 | 16 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2695) | 1:96:A:ASN:HB3 | 1:105:A:ILE:HG23 | 16 | 0.11 |
| (1,2670) | 1:103:A:SER:H | 1:104:A:ASN:HA | 14 | 0.11 |
| (1,2670) | 1:103:A:SER:H | 1:104:A:ASN:HA | 17 | 0.11 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB2 | 2 | 0.11 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB3 | 2 | 0.11 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB2 | 9 | 0.11 |
| (1,2645) | 1:22:A:ALA:HA | 1:100:A:LEU:HB3 | 9 | 0.11 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD11 | 7 | 0.11 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD12 | 7 | 0.11 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD13 | 7 | 0.11 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD21 | 7 | 0.11 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD22 | 7 | 0.11 |
| (1,2628) | 1:100:A:LEU:H | 1:100:A:LEU:HD23 | 7 | 0.11 |
| (1,2610) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HB1 | 10 | 0.11 |
| (1,2610) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HB2 | 10 | 0.11 |
| (1,2610) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HB3 | 10 | 0.11 |
| (1,2610) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HB1 | 10 | 0.11 |
| (1,2610) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HB2 | 10 | 0.11 |
| (1,2610) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HB3 | 10 | 0.11 |
| (1,2609) | 1:23:A:ASN:HD21 | 1:97:A:ALA:HA | 11 | 0.11 |
| (1,2609) | 1:23:A:ASN:HD22 | 1:97:A:ALA:HA | 11 | 0.11 |
| (1,2601) | 1:22:A:ALA:HB1 | 1:96:A:ASN:HA | 4 | 0.11 |
| (1,2601) | 1:22:A:ALA:HB2 | 1:96:A:ASN:HA | 4 | 0.11 |
| (1,2601) | 1:22:A:ALA:HB3 | 1:96:A:ASN:HA | 4 | 0.11 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD11 | 10 | 0.11 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD12 | 10 | 0.11 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD13 | 10 | 0.11 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD21 | 10 | 0.11 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD22 | 10 | 0.11 |
| (1,2573) | 1:92:A:SER:HA | 1:94:A:LEU:HD23 | 10 | 0.11 |
| (1,2558) | 1:21:A:VAL:HG11 | 1:93:A:ALA:HA | 10 | 0.11 |
| (1,2558) | 1:21:A:VAL:HG12 | 1:93:A:ALA:HA | 10 | 0.11 |
| (1,2558) | 1:21:A:VAL:HG13 | 1:93:A:ALA:HA | 10 | 0.11 |
| (1,2558) | 1:21:A:VAL:HG21 | 1:93:A:ALA:HA | 10 | 0.11 |
| (1,2558) | 1:21:A:VAL:HG22 | 1:93:A:ALA:HA | 10 | 0.11 |
| (1,2558) | 1:21:A:VAL:HG23 | 1:93:A:ALA:HA | 10 | 0.11 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE21 | 15 | 0.11 |
| (1,2517) | 1:87:A:ALA:HB1 | 1:88:A:GLN:HE22 | 15 | 0.11 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE21 | 15 | 0.11 |
| (1,2517) | 1:87:A:ALA:HB2 | 1:88:A:GLN:HE22 | 15 | 0.11 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE21 | 15 | 0.11 |
| (1,2517) | 1:87:A:ALA:HB3 | 1:88:A:GLN:HE22 | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,2492) | 1:77:A:LEU:HD11 | 1:86:A:TYR:HA | 14 | 0.11 |
| (1,2492) | 1:77:A:LEU:HD12 | 1:86:A:TYR:HA | 14 | 0.11 |
| (1,2492) | 1:77:A:LEU:HD13 | 1:86:A:TYR:HA | 14 | 0.11 |
| (1,2492) | 1:77:A:LEU:HD21 | 1:86:A:TYR:HA | 14 | 0.11 |
| (1,2492) | 1:77:A:LEU:HD22 | 1:86:A:TYR:HA | 14 | 0.11 |
| (1,2492) | 1:77:A:LEU:HD23 | 1:86:A:TYR:HA | 14 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE1 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG11 | 1:86:A:TYR:HE2 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE1 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG12 | 1:86:A:TYR:HE2 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE1 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG13 | 1:86:A:TYR:HE2 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE1 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG21 | 1:86:A:TYR:HE2 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE1 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG22 | 1:86:A:TYR:HE2 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE1 | 19 | 0.11 |
| (1,2490) | 1:39:A:VAL:HG23 | 1:86:A:TYR:HE2 | 19 | 0.11 |
| (1,2484) | 1:83:A:THR:HG21 | 1:86:A:TYR:H | 1 | 0.11 |
| (1,2484) | 1:83:A:THR:HG22 | 1:86:A:TYR:H | 1 | 0.11 |
| (1,2484) | 1:83:A:THR:HG23 | 1:86:A:TYR:H | 1 | 0.11 |
| (1,2484) | 1:83:A:THR:HG21 | 1:86:A:TYR:H | 18 | 0.11 |
| (1,2484) | 1:83:A:THR:HG22 | 1:86:A:TYR:H | 18 | 0.11 |
| (1,2484) | 1:83:A:THR:HG23 | 1:86:A:TYR:H | 18 | 0.11 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG2 | 2 | 0.11 |
| (1,2444) | 1:77:A:LEU:HG | 1:78:A:PRO:HG3 | 2 | 0.11 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 15 | 0.11 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 15 | 0.11 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 18 | 0.11 |
| (1,2393) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 18 | 0.11 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 15 | 0.11 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 15 | 0.11 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 18 | 0.11 |
| (1,2391) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 18 | 0.11 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 15 | 0.11 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 15 | 0.11 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB2 | 18 | 0.11 |
| (1,2390) | 1:71:A:VAL:HA | 1:75:A:SER:HB3 | 18 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD11 | 1:69:A:PHE:HB2 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD11 | 1:69:A:PHE:HB3 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD12 | 1:69:A:PHE:HB2 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD12 | 1:69:A:PHE:HB3 | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2322) | 1:59:A:LEU:HD13 | 1:69:A:PHE:HB2 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD13 | 1:69:A:PHE:HB3 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD21 | 1:69:A:PHE:HB2 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD21 | 1:69:A:PHE:HB3 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD22 | 1:69:A:PHE:HB2 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD22 | 1:69:A:PHE:HB3 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD23 | 1:69:A:PHE:HB2 | 7 | 0.11 |
| (1,2322) | 1:59:A:LEU:HD23 | 1:69:A:PHE:HB3 | 7 | 0.11 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB2 | 2 | 0.11 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB3 | 2 | 0.11 |
| (1,2287) | 1:66:A:LEU:HD11 | 1:67:A:ALA:HA | 18 | 0.11 |
| (1,2287) | 1:66:A:LEU:HD12 | 1:67:A:ALA:HA | 18 | 0.11 |
| (1,2287) | 1:66:A:LEU:HD13 | 1:67:A:ALA:HA | 18 | 0.11 |
| (1,2287) | 1:66:A:LEU:HD21 | 1:67:A:ALA:HA | 18 | 0.11 |
| (1,2287) | 1:66:A:LEU:HD22 | 1:67:A:ALA:HA | 18 | 0.11 |
| (1,2287) | 1:66:A:LEU:HD23 | 1:67:A:ALA:HA | 18 | 0.11 |
| (1,2280) | 1:62:A:ASP:HA | 1:66:A:LEU:HG | 9 | 0.11 |
| (1,2241) | 1:58:A:THR:HG21 | 1:61:A:VAL:HB | 2 | 0.11 |
| (1,2241) | 1:58:A:THR:HG22 | 1:61:A:VAL:HB | 2 | 0.11 |
| (1,2241) | 1:58:A:THR:HG23 | 1:61:A:VAL:HB | 2 | 0.11 |
| (1,2240) | 1:58:A:THR:HG21 | 1:61:A:VAL:HA | 10 | 0.11 |
| (1,2240) | 1:58:A:THR:HG22 | 1:61:A:VAL:HA | 10 | 0.11 |
| (1,2240) | 1:58:A:THR:HG23 | 1:61:A:VAL:HA | 10 | 0.11 |
| (1,2206) | 1:47:A:VAL:HA | 1:59:A:LEU:HB2 | 16 | 0.11 |
| (1,2206) | 1:47:A:VAL:HA | 1:59:A:LEU:HB3 | 16 | 0.11 |
| (1,2176) | 1:50:A:ARG:HD2 | 1:54:A:SER:HA | 4 | 0.11 |
| (1,2176) | 1:50:A:ARG:HD3 | 1:54:A:SER:HA | 4 | 0.11 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 9 | 0.11 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 9 | 0.11 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 17 | 0.11 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 17 | 0.11 |
| (1,2126) | 1:46:A:SER:HB2 | 1:47:A:VAL:HG11 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB2 | 1:47:A:VAL:HG12 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB2 | 1:47:A:VAL:HG13 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB2 | 1:47:A:VAL:HG21 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB2 | 1:47:A:VAL:HG22 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB2 | 1:47:A:VAL:HG23 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB3 | 1:47:A:VAL:HG11 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB3 | 1:47:A:VAL:HG12 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB3 | 1:47:A:VAL:HG13 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB3 | 1:47:A:VAL:HG21 | 8 | 0.11 |
| (1,2126) | 1:46:A:SER:HB3 | 1:47:A:VAL:HG22 | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2126) | 1:46:A:SER:HB3 | 1:47:A:VAL:HG23 | 8 | 0.11 |
| (1,2112) | 1:41:A:GLN:HE21 | 1:45:A:SER:HA | 3 | 0.11 |
| (1,2112) | 1:41:A:GLN:HE22 | 1:45:A:SER:HA | 3 | 0.11 |
| (1,2112) | 1:41:A:GLN:HE21 | 1:45:A:SER:HA | 9 | 0.11 |
| (1,2112) | 1:41:A:GLN:HE22 | 1:45:A:SER:HA | 9 | 0.11 |
| (1,2105) | 1:41:A:GLN:HB2 | 1:44:A:ALA:HA | 3 | 0.11 |
| (1,2105) | 1:41:A:GLN:HB3 | 1:44:A:ALA:HA | 3 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 2 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 2 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 2 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 2 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 2 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 2 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 6 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 6 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 6 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 6 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 6 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 6 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 8 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 8 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 8 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 8 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 8 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 8 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 15 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 15 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 15 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 15 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 15 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 15 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 19 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 19 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 19 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 19 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 19 | 0.11 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 19 | 0.11 |
| (1,2087) | 1:39:A:VAL:HB | 1:43:A:ILE:HG21 | 20 | 0.11 |
| (1,2087) | 1:39:A:VAL:HB | 1:43:A:ILE:HG22 | 20 | 0.11 |
| (1,2087) | 1:39:A:VAL:HB | 1:43:A:ILE:HG23 | 20 | 0.11 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG21 | 20 | 0.11 |
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG22 | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2086) | 1:40:A:SER:HB2 | 1:43:A:ILE:HG23 | 20 | 0.11 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG21 | 20 | 0.11 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG22 | 20 | 0.11 |
| (1,2086) | 1:40:A:SER:HB3 | 1:43:A:ILE:HG23 | 20 | 0.11 |
| (1,1989) | 1:33:A:THR:HB | 1:34:A:VAL:H | 9 | 0.11 |
| (1,1957) | 1:30:A:THR:HG21 | 1:31:A:LEU:H | 7 | 0.11 |
| (1,1957) | 1:30:A:THR:HG22 | 1:31:A:LEU:H | 7 | 0.11 |
| (1,1957) | 1:30:A:THR:HG23 | 1:31:A:LEU:H | 7 | 0.11 |
| (1,1957) | 1:30:A:THR:HG21 | 1:31:A:LEU:H | 10 | 0.11 |
| (1,1957) | 1:30:A:THR:HG22 | 1:31:A:LEU:H | 10 | 0.11 |
| (1,1957) | 1:30:A:THR:HG23 | 1:31:A:LEU:H | 10 | 0.11 |
| (1,1957) | 1:30:A:THR:HG21 | 1:31:A:LEU:H | 17 | 0.11 |
| (1,1957) | 1:30:A:THR:HG22 | 1:31:A:LEU:H | 17 | 0.11 |
| (1,1957) | 1:30:A:THR:HG23 | 1:31:A:LEU:H | 17 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG11 | 9 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG12 | 9 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG13 | 9 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG21 | 9 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG22 | 9 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG23 | 9 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG11 | 13 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG12 | 13 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG13 | 13 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG21 | 13 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG22 | 13 | 0.11 |
| (1,1895) | 1:17:A:LEU:HG | 1:21:A:VAL:HG23 | 13 | 0.11 |
| (1,1868) | 1:18:A:ILE:HB | 1:19:A:SER:HB2 | 17 | 0.11 |
| (1,1868) | 1:18:A:ILE:HB | 1:19:A:SER:HB3 | 17 | 0.11 |
| (1,1833) | 1:13:A:ALA:HA | 1:16:A:GLY:HA2 | 14 | 0.11 |
| (1,1833) | 1:13:A:ALA:HA | 1:16:A:GLY:HA3 | 14 | 0.11 |
| (1,1823) | 1:4:A:GLN:HA | 1:7:A:PHE:HB2 | 7 | 0.11 |
| (1,1823) | 1:4:A:GLN:HA | 1:7:A:PHE:HB3 | 7 | 0.11 |
| (1,1803) | 1:177:A:THR:H | 1:175:A:PRO:HA | 18 | 0.11 |
| (1,1777) | 1:165:A:SER:H | 1:165:A:SER:HA | 1 | 0.11 |
| (1,1777) | 1:165:A:SER:H | 1:165:A:SER:HA | 4 | 0.11 |
| (1,1707) | 1:149:A:THR:H | 1:149:A:THR:HA | 1 | 0.11 |
| (1,1707) | 1:149:A:THR:H | 1:149:A:THR:HA | 6 | 0.11 |
| (1,1707) | 1:149:A:THR:H | 1:149:A:THR:HA | 18 | 0.11 |
| (1,1660) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 14 | 0.11 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 1 | 0.11 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 7 | 0.11 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 16 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1599) | 1:10:A:THR:H | 1:113:A:LEU:HB2 | 9 | 0.11 |
| (1,1599) | 1:10:A:THR:H | 1:113:A:LEU:HB3 | 9 | 0.11 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 5 | 0.11 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 9 | 0.11 |
| (1,1578) | 1:105:A:ILE:HA | 1:107:A:THR:H | 16 | 0.11 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD2 | 2 | 0.11 |
| (1,1354) | 1:50:A:ARG:H | 1:50:A:ARG:HD3 | 2 | 0.11 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 9 | 0.11 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 9 | 0.11 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 17 | 0.11 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 17 | 0.11 |
| (1,1281) | 1:33:A:THR:HB | 1:34:A:VAL:H | 9 | 0.11 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB2 | 20 | 0.11 |
| (1,1167) | 1:139:A:ASP:H | 1:135:A:SER:HB3 | 20 | 0.11 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG11 | 6 | 0.11 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG12 | 6 | 0.11 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG13 | 6 | 0.11 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG21 | 6 | 0.11 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG22 | 6 | 0.11 |
| (1,1162) | 1:46:A:SER:H | 1:48:A:VAL:HG23 | 6 | 0.11 |
| (1,1157) | 1:121:A:SER:H | 1:123:A:ALA:HB1 | 14 | 0.11 |
| (1,1157) | 1:121:A:SER:H | 1:123:A:ALA:HB2 | 14 | 0.11 |
| (1,1157) | 1:121:A:SER:H | 1:123:A:ALA:HB3 | 14 | 0.11 |
| (1,1156) | 1:34:A:VAL:H | 1:34:A:VAL:HA | 4 | 0.11 |
| (1,1156) | 1:34:A:VAL:H | 1:34:A:VAL:HA | 8 | 0.11 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG11 | 1 | 0.11 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG12 | 1 | 0.11 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG13 | 1 | 0.11 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG21 | 1 | 0.11 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG22 | 1 | 0.11 |
| (1,1145) | 1:127:A:LEU:H | 1:120:A:VAL:HG23 | 1 | 0.11 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG21 | 13 | 0.11 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG22 | 13 | 0.11 |
| (1,1136) | 1:19:A:SER:H | 1:18:A:ILE:HG23 | 13 | 0.11 |
| (1,1132) | 1:135:A:SER:H | 1:135:A:SER:HA | 18 | 0.11 |
| (1,1087) | 1:64:A:ASN:H | 1:66:A:LEU:HA | 12 | 0.11 |
| (1,1075) | 1:48:A:VAL:H | 1:73:A:ALA:HB1 | 10 | 0.11 |
| (1,1075) | 1:48:A:VAL:H | 1:73:A:ALA:HB2 | 10 | 0.11 |
| (1,1075) | 1:48:A:VAL:H | 1:73:A:ALA:HB3 | 10 | 0.11 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG21 | 2 | 0.11 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG22 | 2 | 0.11 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HG23 | 2 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD11 | 3 | 0.11 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD12 | 3 | 0.11 |
| (1,1071) | 1:108:A:LEU:H | 1:105:A:ILE:HD13 | 3 | 0.11 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG11 | 17 | 0.11 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG12 | 17 | 0.11 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG13 | 17 | 0.11 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG21 | 17 | 0.11 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG22 | 17 | 0.11 |
| (1,1070) | 1:67:A:ALA:H | 1:71:A:VAL:HG23 | 17 | 0.11 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA2 | 13 | 0.11 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA3 | 13 | 0.11 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 5 | 0.11 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 17 | 0.11 |
| (1,1028) | 1:71:A:VAL:H | 1:66:A:LEU:HA | 16 | 0.11 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 5 | 0.11 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 10 | 0.11 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 13 | 0.11 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 14 | 0.11 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 15 | 0.11 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 17 | 0.11 |
| (1,1002) | 1:92:A:SER:H | 1:21:A:VAL:HB | 20 | 0.11 |
| (1,946) | 1:196:A:GLY:H | 1:197:A:PHE:HA | 9 | 0.11 |
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG2 | 10 | 0.11 |
| (1,933) | 1:20:A:ARG:H | 1:191:A:PRO:HG3 | 10 | 0.11 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD2 | 1 | 0.11 |
| (1,923) | 1:182:A:TYR:H | 1:185:A:PRO:HD3 | 1 | 0.11 |
| (1,917) | 1:161:A:ALA:H | 1:177:A:THR:HB | 18 | 0.11 |
| (1,913) | 1:169:A:TYR:H | 1:175:A:PRO:HD2 | 12 | 0.11 |
| (1,913) | 1:169:A:TYR:H | 1:175:A:PRO:HD3 | 12 | 0.11 |
| (1,913) | 1:169:A:TYR:H | 1:175:A:PRO:HD2 | 17 | 0.11 |
| (1,913) | 1:169:A:TYR:H | 1:175:A:PRO:HD3 | 17 | 0.11 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG2 | 4 | 0.11 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG3 | 4 | 0.11 |
| (1,885) | 1:154:A:ALA:HA | 1:156:A:TYR:H | 19 | 0.11 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB2 | 19 | 0.11 |
| (1,878) | 1:153:A:SER:H | 1:153:A:SER:HB3 | 19 | 0.11 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB2 | 9 | 0.11 |
| (1,877) | 1:147:A:LEU:H | 1:150:A:SER:HB3 | 9 | 0.11 |
| (1,860) | 1:28:A:THR:H | 1:144:A:SER:HB2 | 3 | 0.11 |
| (1,860) | 1:28:A:THR:H | 1:144:A:SER:HB3 | 3 | 0.11 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 6 | 0.11 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 3 | 0.11 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 3 | 0.11 |
| (1,824) | 1:37:A:THR:HG21 | 1:136:A:VAL:H | 7 | 0.11 |
| (1,824) | 1:37:A:THR:HG22 | 1:136:A:VAL:H | 7 | 0.11 |
| (1,824) | 1:37:A:THR:HG23 | 1:136:A:VAL:H | 7 | 0.11 |
| (1,824) | 1:37:A:THR:HG21 | 1:136:A:VAL:H | 15 | 0.11 |
| (1,824) | 1:37:A:THR:HG22 | 1:136:A:VAL:H | 15 | 0.11 |
| (1,824) | 1:37:A:THR:HG23 | 1:136:A:VAL:H | 15 | 0.11 |
| (1,801) | 1:131:A:VAL:HB | 1:132:A:ASP:H | 14 | 0.11 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 5 | 0.11 |
| (1,783) | 1:50:A:ARG:HD2 | 1:129:A:ILE:H | 11 | 0.11 |
| (1,783) | 1:50:A:ARG:HD3 | 1:129:A:ILE:H | 11 | 0.11 |
| (1,734) | 1:118:A:ASN:HA | 1:121:A:SER:H | 7 | 0.11 |
| (1,728) | 1:116:A:LEU:H | 1:120:A:VAL:H | 3 | 0.11 |
| (1,728) | 1:116:A:LEU:H | 1:120:A:VAL:H | 12 | 0.11 |
| (1,671) | 1:10:A:THR:H | 1:113:A:LEU:HB2 | 9 | 0.11 |
| (1,671) | 1:10:A:THR:H | 1:113:A:LEU:HB3 | 9 | 0.11 |
| (1,648) | 1:108:A:LEU:HD11 | 1:110:A:SER:H | 3 | 0.11 |
| (1,648) | 1:108:A:LEU:HD12 | 1:110:A:SER:H | 3 | 0.11 |
| (1,648) | 1:108:A:LEU:HD13 | 1:110:A:SER:H | 3 | 0.11 |
| (1,648) | 1:108:A:LEU:HD21 | 1:110:A:SER:H | 3 | 0.11 |
| (1,648) | 1:108:A:LEU:HD22 | 1:110:A:SER:H | 3 | 0.11 |
| (1,648) | 1:108:A:LEU:HD23 | 1:110:A:SER:H | 3 | 0.11 |
| (1,648) | 1:108:A:LEU:HD11 | 1:110:A:SER:H | 6 | 0.11 |
| (1,648) | 1:108:A:LEU:HD12 | 1:110:A:SER:H | 6 | 0.11 |
| (1,648) | 1:108:A:LEU:HD13 | 1:110:A:SER:H | 6 | 0.11 |
| (1,648) | 1:108:A:LEU:HD21 | 1:110:A:SER:H | 6 | 0.11 |
| (1,648) | 1:108:A:LEU:HD22 | 1:110:A:SER:H | 6 | 0.11 |
| (1,648) | 1:108:A:LEU:HD23 | 1:110:A:SER:H | 6 | 0.11 |
| (1,598) | 1:96:A:ASN:HD21 | 1:104:A:ASN:HD21 | 9 | 0.11 |
| (1,598) | 1:96:A:ASN:HD21 | 1:104:A:ASN:HD22 | 9 | 0.11 |
| (1,598) | 1:96:A:ASN:HD22 | 1:104:A:ASN:HD21 | 9 | 0.11 |
| (1,598) | 1:96:A:ASN:HD22 | 1:104:A:ASN:HD22 | 9 | 0.11 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD21 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG11 | 1:104:A:ASN:HD22 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD21 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG12 | 1:104:A:ASN:HD22 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD21 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG13 | 1:104:A:ASN:HD22 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD21 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG21 | 1:104:A:ASN:HD22 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD21 | 11 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,597) | 1:21:A:VAL:HG22 | 1:104:A:ASN:HD22 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD21 | 11 | 0.11 |
| (1,597) | 1:21:A:VAL:HG23 | 1:104:A:ASN:HD22 | 11 | 0.11 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD21 | 19 | 0.11 |
| (1,588) | 1:101:A:ASN:H | 1:104:A:ASN:HD22 | 19 | 0.11 |
| (1,524) | 1:37:A:THR:H | 1:95:A:PHE:HB2 | 5 | 0.11 |
| (1,524) | 1:37:A:THR:H | 1:95:A:PHE:HB3 | 5 | 0.11 |
| (1,455) | 1:83:A:THR:HG21 | 1:84:A:SER:H | 1 | 0.11 |
| (1,455) | 1:83:A:THR:HG22 | 1:84:A:SER:H | 1 | 0.11 |
| (1,455) | 1:83:A:THR:HG23 | 1:84:A:SER:H | 1 | 0.11 |
| (1,455) | 1:83:A:THR:HG21 | 1:84:A:SER:H | 18 | 0.11 |
| (1,455) | 1:83:A:THR:HG22 | 1:84:A:SER:H | 18 | 0.11 |
| (1,455) | 1:83:A:THR:HG23 | 1:84:A:SER:H | 18 | 0.11 |
| (1,352) | 1:66:A:LEU:HG | 1:67:A:ALA:H | 19 | 0.11 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB2 | 10 | 0.11 |
| (1,331) | 1:62:A:ASP:H | 1:64:A:ASN:HB3 | 10 | 0.11 |
| (1,323) | 1:61:A:VAL:HA | 1:63:A:GLY:H | 7 | 0.11 |
| (1,295) | 1:50:A:ARG:HB2 | 1:57:A:SER:H | 7 | 0.11 |
| (1,295) | 1:50:A:ARG:HB3 | 1:57:A:SER:H | 7 | 0.11 |
| (1,276) | 1:50:A:ARG:HB2 | 1:54:A:SER:H | 17 | 0.11 |
| (1,276) | 1:50:A:ARG:HB3 | 1:54:A:SER:H | 17 | 0.11 |
| (1,268) | 1:50:A:ARG:HG2 | 1:53:A:GLN:H | 5 | 0.11 |
| (1,268) | 1:50:A:ARG:HG3 | 1:53:A:GLN:H | 5 | 0.11 |
| (1,258) | 1:49:A:GLN:HB2 | 1:51:A:ALA:H | 3 | 0.11 |
| (1,258) | 1:49:A:GLN:HB3 | 1:51:A:ALA:H | 3 | 0.11 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB2 | 4 | 0.11 |
| (1,203) | 1:10:A:THR:H | 1:42:A:GLN:HB3 | 4 | 0.11 |
| (1,192) | 1:36:A:ARG:HG2 | 1:40:A:SER:H | 3 | 0.11 |
| (1,192) | 1:36:A:ARG:HG3 | 1:40:A:SER:H | 3 | 0.11 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 1 | 0.11 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 11 | 0.11 |
| (1,106) | 1:27:A:ASN:H | 1:27:A:ASN:HD21 | 18 | 0.11 |
| (1,106) | 1:27:A:ASN:H | 1:27:A:ASN:HD22 | 18 | 0.11 |
| (1,43) | 1:18:A:ILE:HG12 | 1:19:A:SER:H | 1 | 0.11 |
| (1,43) | 1:18:A:ILE:HG13 | 1:19:A:SER:H | 1 | 0.11 |
| (1,6) | 1:6:A:GLY:HA2 | 1:7:A:PHE:H | 1 | 0.11 |
| (1,6) | 1:6:A:GLY:HA3 | 1:7:A:PHE:H | 1 | 0.11 |
| (1,6) | 1:6:A:GLY:HA2 | 1:7:A:PHE:H | 5 | 0.11 |
| (1,6) | 1:6:A:GLY:HA3 | 1:7:A:PHE:H | 5 | 0.11 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE1 | 18 | 0.1 |
| (1,3892) | 1:37:A:THR:HG21 | 1:95:A:PHE:HE2 | 18 | 0.1 |
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE1 | 18 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3892) | 1:37:A:THR:HG22 | 1:95:A:PHE:HE2 | 18 | 0.1 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE1 | 18 | 0.1 |
| (1,3892) | 1:37:A:THR:HG23 | 1:95:A:PHE:HE2 | 18 | 0.1 |
| (1,3796) | 1:124:A:ALA:HB1 | 1:120:A:VAL:HA | 15 | 0.1 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG2 | 10 | 0.1 |
| (1,3781) | 1:21:A:VAL:HG23 | 1:20:A:ARG:HG3 | 10 | 0.1 |
| (1,3683) | 1:56:A:ALA:HB2 | 1:50:A:ARG:HA | 18 | 0.1 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB2 | 5 | 0.1 |
| (1,3639) | 1:156:A:TYR:HB3 | 1:157:A:SER:HB3 | 5 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD11 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD12 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD13 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD21 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD22 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE1 | 1:116:A:LEU:HD23 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD11 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD12 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD13 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD21 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD22 | 20 | 0.1 |
| (1,3607) | 1:90:A:PHE:HE2 | 1:116:A:LEU:HD23 | 20 | 0.1 |
| (1,3545) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB2 | 17 | 0.1 |
| (1,3545) | 1:48:A:VAL:HG13 | 1:41:A:GLN:HB3 | 17 | 0.1 |
| (1,3543) | 1:17:A:LEU:HD11 | 1:93:A:ALA:HA | 18 | 0.1 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD2 | 20 | 0.1 |
| (1,3519) | 1:17:A:LEU:HB2 | 1:20:A:ARG:HD3 | 20 | 0.1 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD2 | 20 | 0.1 |
| (1,3519) | 1:17:A:LEU:HB3 | 1:20:A:ARG:HD3 | 20 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD11 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD12 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD13 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD21 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD22 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD21 | 1:17:A:LEU:HD23 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD11 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD12 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD13 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD21 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD22 | 1 | 0.1 |
| (1,3511) | 1:96:A:ASN:HD22 | 1:17:A:LEU:HD23 | 1 | 0.1 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB2 | 8 | 0.1 |
| (1,3422) | 1:35:A:LEU:HD13 | 1:86:A:TYR:HB3 | 8 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD11 | 11 | 0.1 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD12 | 11 | 0.1 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD13 | 11 | 0.1 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD21 | 11 | 0.1 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD22 | 11 | 0.1 |
| (1,3401) | 1:36:A:ARG:HB3 | 1:94:A:LEU:HD23 | 11 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 16 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 16 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 16 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 16 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 16 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 16 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG11 | 18 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG12 | 18 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG13 | 18 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG21 | 18 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG22 | 18 | 0.1 |
| (1,3222) | 1:43:A:ILE:HB | 1:39:A:VAL:HG23 | 18 | 0.1 |
| (1,3207) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB2 | 19 | 0.1 |
| (1,3207) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB3 | 19 | 0.1 |
| (1,3207) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB2 | 19 | 0.1 |
| (1,3207) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB3 | 19 | 0.1 |
| (1,3206) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB2 | 19 | 0.1 |
| (1,3206) | 1:194:A:GLN:HG2 | 1:197:A:PHE:HB3 | 19 | 0.1 |
| (1,3206) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB2 | 19 | 0.1 |
| (1,3206) | 1:194:A:GLN:HG3 | 1:197:A:PHE:HB3 | 19 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3200) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG11 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG12 | 1:194:A:GLN:HG3 | 17 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,3199) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG13 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG21 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG22 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG2 | 17 | 0.1 |
| (1,3199) | 1:99:A:VAL:HG23 | 1:194:A:GLN:HG3 | 17 | 0.1 |
| (1,3135) | 1:170:A:THR:HB | 1:175:A:PRO:HD2 | 13 | 0.1 |
| (1,3135) | 1:170:A:THR:HB | 1:175:A:PRO:HD3 | 13 | 0.1 |
| (1,3135) | 1:170:A:THR:HB | 1:175:A:PRO:HD2 | 19 | 0.1 |
| (1,3135) | 1:170:A:THR:HB | 1:175:A:PRO:HD3 | 19 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD2 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD11 | 1:172:A:PRO:HD3 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD2 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD12 | 1:172:A:PRO:HD3 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD2 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD13 | 1:172:A:PRO:HD3 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD2 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD21 | 1:172:A:PRO:HD3 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD2 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD22 | 1:172:A:PRO:HD3 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD2 | 17 | 0.1 |
| (1,3124) | 1:31:A:LEU:HD23 | 1:172:A:PRO:HD3 | 17 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG21 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG22 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB1 | 1:170:A:THR:HG23 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG21 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG22 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB2 | 1:170:A:THR:HG23 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG21 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG22 | 8 | 0.1 |
| (1,3120) | 1:167:A:ALA:HB3 | 1:170:A:THR:HG23 | 8 | 0.1 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG2 | 4 | 0.1 |
| (1,3103) | 1:157:A:SER:HB2 | 1:158:A:GLN:HG3 | 4 | 0.1 |
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG2 | 4 | 0.1 |
| (1,3103) | 1:157:A:SER:HB3 | 1:158:A:GLN:HG3 | 4 | 0.1 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB1 | 16 | 0.1 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB2 | 16 | 0.1 |
| (1,3096) | 1:148:A:SER:HA | 1:154:A:ALA:HB3 | 16 | 0.1 |
| (1,3087) | 1:148:A:SER:HB2 | 1:149:A:THR:HB | 20 | 0.1 |
| (1,3087) | 1:148:A:SER:HB3 | 1:149:A:THR:HB | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3005) | 1:37:A:THR:HG21 | 1:136:A:VAL:HA | 1 | 0.1 |
| (1,3005) | 1:37:A:THR:HG22 | 1:136:A:VAL:HA | 1 | 0.1 |
| (1,3005) | 1:37:A:THR:HG23 | 1:136:A:VAL:HA | 1 | 0.1 |
| (1,3005) | 1:37:A:THR:HG21 | 1:136:A:VAL:HA | 13 | 0.1 |
| (1,3005) | 1:37:A:THR:HG22 | 1:136:A:VAL:HA | 13 | 0.1 |
| (1,3005) | 1:37:A:THR:HG23 | 1:136:A:VAL:HA | 13 | 0.1 |
| (1,3003) | 1:131:A:VAL:HG11 | 1:136:A:VAL:HB | 14 | 0.1 |
| (1,3003) | 1:131:A:VAL:HG12 | 1:136:A:VAL:HB | 14 | 0.1 |
| (1,3003) | 1:131:A:VAL:HG13 | 1:136:A:VAL:HB | 14 | 0.1 |
| (1,3003) | 1:131:A:VAL:HG21 | 1:136:A:VAL:HB | 14 | 0.1 |
| (1,3003) | 1:131:A:VAL:HG22 | 1:136:A:VAL:HB | 14 | 0.1 |
| (1,3003) | 1:131:A:VAL:HG23 | 1:136:A:VAL:HB | 14 | 0.1 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA2 | 9 | 0.1 |
| (1,2981) | 1:71:A:VAL:HB | 1:134:A:GLY:HA3 | 9 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB2 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG11 | 1:133:A:SER:HB3 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB2 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG12 | 1:133:A:SER:HB3 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB2 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG13 | 1:133:A:SER:HB3 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB2 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG21 | 1:133:A:SER:HB3 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB2 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG22 | 1:133:A:SER:HB3 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB2 | 1 | 0.1 |
| (1,2979) | 1:136:A:VAL:HG23 | 1:133:A:SER:HB3 | 1 | 0.1 |
| (1,2864) | 1:117:A:LEU:HG | 1:120:A:VAL:HB | 13 | 0.1 |
| (1,2835) | 1:110:A:SER:HA | 1:117:A:LEU:HA | 16 | 0.1 |
| (1,2783) | 1:7:A:PHE:HA | 1:114:A:SER:HB2 | 6 | 0.1 |
| (1,2783) | 1:7:A:PHE:HA | 1:114:A:SER:HB3 | 6 | 0.1 |
| (1,2693) | 1:104:A:ASN:HB2 | 1:105:A:ILE:HD11 | 20 | 0.1 |
| (1,2693) | 1:104:A:ASN:HB2 | 1:105:A:ILE:HD12 | 20 | 0.1 |
| (1,2693) | 1:104:A:ASN:HB2 | 1:105:A:ILE:HD13 | 20 | 0.1 |
| (1,2693) | 1:104:A:ASN:HB3 | 1:105:A:ILE:HD11 | 20 | 0.1 |
| (1,2693) | 1:104:A:ASN:HB3 | 1:105:A:ILE:HD12 | 20 | 0.1 |
| (1,2693) | 1:104:A:ASN:HB3 | 1:105:A:ILE:HD13 | 20 | 0.1 |
| (1,2671) | 1:103:A:SER:H | 1:104:A:ASN:HB2 | 11 | 0.1 |
| (1,2671) | 1:103:A:SER:H | 1:104:A:ASN:HB3 | 11 | 0.1 |
| (1,2670) | 1:103:A:SER:H | 1:104:A:ASN:HA | 19 | 0.1 |
| (1,2669) | 1:103:A:SER:H | 1:104:A:ASN:HB2 | 11 | 0.1 |
| (1,2669) | 1:103:A:SER:H | 1:104:A:ASN:HB3 | 11 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2647) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG11 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD11 | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG12 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG13 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG21 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG22 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD11 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD12 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD13 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD21 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD22 | 20 | 0.1 |
| (1,2646) | 1:21:A:VAL:HG23 | 1:100:A:LEU:HD23 | 20 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG11 | 2 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG12 | 2 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG13 | 2 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG21 | 2 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG22 | 2 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG23 | 2 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG11 | 3 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG12 | 3 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG13 | 3 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG21 | 3 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG22 | 3 | 0.1 |
| (1,2621) | 1:98:A:GLY:H | 1:99:A:VAL:HG23 | 3 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB1 | 9 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB2 | 9 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB3 | 9 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB1 | 9 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB2 | 9 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB3 | 9 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB1 | 15 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB2 | 15 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB2 | 1:97:A:ALA:HB3 | 15 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB1 | 15 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB2 | 15 | 0.1 |
| (1,2607) | 1:96:A:ASN:HB3 | 1:97:A:ALA:HB3 | 15 | 0.1 |
| (1,2601) | 1:22:A:ALA:HB1 | 1:96:A:ASN:HA | 3 | 0.1 |
| (1,2601) | 1:22:A:ALA:HB2 | 1:96:A:ASN:HA | 3 | 0.1 |
| (1,2601) | 1:22:A:ALA:HB3 | 1:96:A:ASN:HA | 3 | 0.1 |
| (1,2600) | 1:93:A:ALA:HB1 | 1:96:A:ASN:HB2 | 14 | 0.1 |
| (1,2600) | 1:93:A:ALA:HB1 | 1:96:A:ASN:HB3 | 14 | 0.1 |
| (1,2600) | 1:93:A:ALA:HB2 | 1:96:A:ASN:HB2 | 14 | 0.1 |
| (1,2600) | 1:93:A:ALA:HB2 | 1:96:A:ASN:HB3 | 14 | 0.1 |
| (1,2600) | 1:93:A:ALA:HB3 | 1:96:A:ASN:HB2 | 14 | 0.1 |
| (1,2600) | 1:93:A:ALA:HB3 | 1:96:A:ASN:HB3 | 14 | 0.1 |
| (1,2591) | 1:23:A:ASN:HD21 | 1:95:A:PHE:HD1 | 16 | 0.1 |
| (1,2591) | 1:23:A:ASN:HD21 | 1:95:A:PHE:HD2 | 16 | 0.1 |
| (1,2591) | 1:23:A:ASN:HD22 | 1:95:A:PHE:HD1 | 16 | 0.1 |
| (1,2591) | 1:23:A:ASN:HD22 | 1:95:A:PHE:HD2 | 16 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD11 | 1:91:A:SER:HB2 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD11 | 1:91:A:SER:HB3 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD12 | 1:91:A:SER:HB2 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD12 | 1:91:A:SER:HB3 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD13 | 1:91:A:SER:HB2 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD13 | 1:91:A:SER:HB3 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD21 | 1:91:A:SER:HB2 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD21 | 1:91:A:SER:HB3 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD22 | 1:91:A:SER:HB2 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD22 | 1:91:A:SER:HB3 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD23 | 1:91:A:SER:HB2 | 14 | 0.1 |
| (1,2542) | 1:31:A:LEU:HD23 | 1:91:A:SER:HB3 | 14 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD11 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD12 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD13 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD21 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD22 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD2 | 1:77:A:LEU:HD23 | 6 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD11 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD12 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD13 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD21 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD22 | 6 | 0.1 |
| (1,2416) | 1:76:A:ARG:HD3 | 1:77:A:LEU:HD23 | 6 | 0.1 |
| (1,2387) | 1:75:A:SER:H | 1:75:A:SER:HA | 9 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD11 | 1:69:A:PHE:HB2 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD11 | 1:69:A:PHE:HB3 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD12 | 1:69:A:PHE:HB2 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD12 | 1:69:A:PHE:HB3 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD13 | 1:69:A:PHE:HB2 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD13 | 1:69:A:PHE:HB3 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD21 | 1:69:A:PHE:HB2 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD21 | 1:69:A:PHE:HB3 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD22 | 1:69:A:PHE:HB2 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD22 | 1:69:A:PHE:HB3 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD23 | 1:69:A:PHE:HB2 | 17 | 0.1 |
| (1,2322) | 1:59:A:LEU:HD23 | 1:69:A:PHE:HB3 | 17 | 0.1 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB2 | 12 | 0.1 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB3 | 12 | 0.1 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB2 | 15 | 0.1 |
| (1,2320) | 1:65:A:ASN:H | 1:69:A:PHE:HB3 | 15 | 0.1 |
| (1,2280) | 1:62:A:ASP:HA | 1:66:A:LEU:HG | 14 | 0.1 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD21 | 3 | 0.1 |
| (1,2263) | 1:60:A:GLY:HA2 | 1:64:A:ASN:HD22 | 3 | 0.1 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD21 | 3 | 0.1 |
| (1,2263) | 1:60:A:GLY:HA3 | 1:64:A:ASN:HD22 | 3 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG21 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG22 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG11 | 1:58:A:THR:HG23 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG21 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG22 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG12 | 1:58:A:THR:HG23 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG21 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG22 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG13 | 1:58:A:THR:HG23 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG21 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG22 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG21 | 1:58:A:THR:HG23 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG21 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG22 | 8 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,2219) | 1:47:A:VAL:HG22 | 1:58:A:THR:HG23 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG21 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG22 | 8 | 0.1 |
| (1,2219) | 1:47:A:VAL:HG23 | 1:58:A:THR:HG23 | 8 | 0.1 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB2 | 15 | 0.1 |
| (1,2210) | 1:54:A:SER:HA | 1:57:A:SER:HB3 | 15 | 0.1 |
| (1,2206) | 1:47:A:VAL:HA | 1:59:A:LEU:HB2 | 17 | 0.1 |
| (1,2206) | 1:47:A:VAL:HA | 1:59:A:LEU:HB3 | 17 | 0.1 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 2 | 0.1 |
| (1,2147) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 2 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 16 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 16 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 16 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 16 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 16 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 16 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG11 | 1:43:A:ILE:HB | 18 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG12 | 1:43:A:ILE:HB | 18 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG13 | 1:43:A:ILE:HB | 18 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG21 | 1:43:A:ILE:HB | 18 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG22 | 1:43:A:ILE:HB | 18 | 0.1 |
| (1,2090) | 1:39:A:VAL:HG23 | 1:43:A:ILE:HB | 18 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG21 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG22 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG23 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG21 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG22 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG23 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG21 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG22 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG23 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG21 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG22 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG23 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG21 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG22 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG23 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG21 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG22 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG23 | 8 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG21 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG22 | 13 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,2017) | 1:35:A:LEU:HD11 | 1:37:A:THR:HG23 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG21 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG22 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD12 | 1:37:A:THR:HG23 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG21 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG22 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD13 | 1:37:A:THR:HG23 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG21 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG22 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD21 | 1:37:A:THR:HG23 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG21 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG22 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD22 | 1:37:A:THR:HG23 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG21 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG22 | 13 | 0.1 |
| (1,2017) | 1:35:A:LEU:HD23 | 1:37:A:THR:HG23 | 13 | 0.1 |
| (1,1989) | 1:33:A:THR:HB | 1:34:A:VAL:H | 16 | 0.1 |
| (1,1976) | 1:32:A:ARG:HG2 | 1:33:A:THR:HA | 4 | 0.1 |
| (1,1976) | 1:32:A:ARG:HG3 | 1:33:A:THR:HA | 4 | 0.1 |
| (1,1904) | 1:20:A:ARG:HA | 1:24:A:ALA:HA | 7 | 0.1 |
| (1,1807) | 1:150:A:SER:H | 1:150:A:SER:HA | 6 | 0.1 |
| (1,1736) | 1:176:A:SER:HA | 1:177:A:THR:H | 8 | 0.1 |
| (1,1652) | 1:131:A:VAL:H | 1:131:A:VAL:HA | 9 | 0.1 |
| (1,1551) | 1:99:A:VAL:HB | 1:100:A:LEU:H | 4 | 0.1 |
| (1,1411) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 10 | 0.1 |
| (1,1403) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 10 | 0.1 |
| (1,1403) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 10 | 0.1 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG2 | 2 | 0.1 |
| (1,1352) | 1:50:A:ARG:H | 1:50:A:ARG:HG3 | 2 | 0.1 |
| (1,1281) | 1:33:A:THR:HB | 1:34:A:VAL:H | 16 | 0.1 |
| (1,1257) | 1:27:A:ASN:H | 1:27:A:ASN:HB2 | 10 | 0.1 |
| (1,1257) | 1:27:A:ASN:H | 1:27:A:ASN:HB3 | 10 | 0.1 |
| (1,1181) | 1:56:A:ALA:H | 1:58:A:THR:HG21 | 4 | 0.1 |
| (1,1181) | 1:56:A:ALA:H | 1:58:A:THR:HG22 | 4 | 0.1 |
| (1,1181) | 1:56:A:ALA:H | 1:58:A:THR:HG23 | 4 | 0.1 |
| (1,1166) | 1:97:A:ALA:H | 1:97:A:ALA:HA | 4 | 0.1 |
| (1,1156) | 1:34:A:VAL:H | 1:34:A:VAL:HA | 15 | 0.1 |
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG12 | 4 | 0.1 |
| (1,1070) | 1:52:A:ALA:H | 1:129:A:ILE:HG13 | 4 | 0.1 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA2 | 6 | 0.1 |
| (1,1066) | 1:174:A:GLY:H | 1:171:A:GLY:HA3 | 6 | 0.1 |
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 7 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1037) | 1:173:A:SER:H | 1:173:A:SER:HA | 19 | 0.1 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD11 | 9 | 0.1 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD12 | 9 | 0.1 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD13 | 9 | 0.1 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD21 | 9 | 0.1 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD22 | 9 | 0.1 |
| (1,1034) | 1:109:A:GLY:H | 1:113:A:LEU:HD23 | 9 | 0.1 |
| (1,1030) | 1:65:A:ASN:H | 1:65:A:ASN:HA | 13 | 0.1 |
| (1,1030) | 1:65:A:ASN:H | 1:65:A:ASN:HA | 20 | 0.1 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 1 | 0.1 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 6 | 0.1 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 8 | 0.1 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 12 | 0.1 |
| (1,1012) | 1:146:A:PHE:H | 1:146:A:PHE:HA | 18 | 0.1 |
| (1,989) | 1:110:A:SER:H | 1:117:A:LEU:HG | 19 | 0.1 |
| (1,949) | 1:55:A:LEU:H | 1:129:A:ILE:HD11 | 15 | 0.1 |
| (1,949) | 1:55:A:LEU:H | 1:129:A:ILE:HD12 | 15 | 0.1 |
| (1,949) | 1:55:A:LEU:H | 1:129:A:ILE:HD13 | 15 | 0.1 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG2 | 11 | 0.1 |
| (1,911) | 1:20:A:ARG:HE | 1:172:A:PRO:HG3 | 11 | 0.1 |
| (1,897) | 1:156:A:TYR:HA | 1:160:A:SER:H | 10 | 0.1 |
| (1,851) | 1:137:A:GLN:HB2 | 1:141:A:SER:H | 12 | 0.1 |
| (1,851) | 1:137:A:GLN:HB3 | 1:141:A:SER:H | 12 | 0.1 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE21 | 5 | 0.1 |
| (1,832) | 1:136:A:VAL:H | 1:137:A:GLN:HE22 | 5 | 0.1 |
| (1,788) | 1:129:A:ILE:HB | 1:130:A:ASN:H | 11 | 0.1 |
| (1,682) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB1 | 6 | 0.1 |
| (1,682) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB2 | 6 | 0.1 |
| (1,682) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB3 | 6 | 0.1 |
| (1,682) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB1 | 6 | 0.1 |
| (1,682) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB2 | 6 | 0.1 |
| (1,682) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB3 | 6 | 0.1 |
| (1,681) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB1 | 6 | 0.1 |
| (1,681) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB2 | 6 | 0.1 |
| (1,681) | 1:42:A:GLN:HE21 | 1:115:A:ALA:HB3 | 6 | 0.1 |
| (1,681) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB1 | 6 | 0.1 |
| (1,681) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB2 | 6 | 0.1 |
| (1,681) | 1:42:A:GLN:HE22 | 1:115:A:ALA:HB3 | 6 | 0.1 |
| (1,633) | 1:14:A:SER:H | 1:108:A:LEU:HB2 | 9 | 0.1 |
| (1,633) | 1:14:A:SER:H | 1:108:A:LEU:HB3 | 9 | 0.1 |
| (1,609) | 1:101:A:ASN:H | 1:105:A:ILE:H | 20 | 0.1 |
| (1,580) | 1:104:A:ASN:HB2 | 1:103:A:SER:H | 11 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,580) | 1:104:A:ASN:HB3 | 1:103:A:SER:H | 11 | 0.1 |
| (1,559) | 1:99:A:VAL:HB | 1:100:A:LEU:H | 4 | 0.1 |
| (1,531) | 1:95:A:PHE:HD1 | 1:96:A:ASN:H | 12 | 0.1 |
| (1,531) | 1:95:A:PHE:HD2 | 1:96:A:ASN:H | 12 | 0.1 |
| (1,474) | 1:88:A:GLN:H | 1:88:A:GLN:HA | 16 | 0.1 |
| (1,388) | 1:70:A:ALA:H | 1:72:A:GLN:H | 9 | 0.1 |
| (1,340) | 1:60:A:GLY:H | 1:65:A:ASN:HD21 | 10 | 0.1 |
| (1,340) | 1:60:A:GLY:H | 1:65:A:ASN:HD22 | 10 | 0.1 |
| (1,332) | 1:61:A:VAL:HA | 1:64:A:ASN:H | 7 | 0.1 |
| (1,320) | 1:62:A:ASP:HA | 1:63:A:GLY:H | 10 | 0.1 |
| (1,315) | 1:53:A:GLN:HE21 | 1:61:A:VAL:HB | 10 | 0.1 |
| (1,315) | 1:53:A:GLN:HE22 | 1:61:A:VAL:HB | 10 | 0.1 |
| (1,295) | 1:50:A:ARG:HB2 | 1:57:A:SER:H | 10 | 0.1 |
| (1,295) | 1:50:A:ARG:HB3 | 1:57:A:SER:H | 10 | 0.1 |
| (1,291) | 1:55:A:LEU:HD11 | 1:57:A:SER:H | 10 | 0.1 |
| (1,291) | 1:55:A:LEU:HD12 | 1:57:A:SER:H | 10 | 0.1 |
| (1,291) | 1:55:A:LEU:HD13 | 1:57:A:SER:H | 10 | 0.1 |
| (1,291) | 1:55:A:LEU:HD21 | 1:57:A:SER:H | 10 | 0.1 |
| (1,291) | 1:55:A:LEU:HD22 | 1:57:A:SER:H | 10 | 0.1 |
| (1,291) | 1:55:A:LEU:HD23 | 1:57:A:SER:H | 10 | 0.1 |
| (1,276) | 1:50:A:ARG:HB2 | 1:54:A:SER:H | 2 | 0.1 |
| (1,276) | 1:50:A:ARG:HB3 | 1:54:A:SER:H | 2 | 0.1 |
| (1,276) | 1:50:A:ARG:HB2 | 1:54:A:SER:H | 19 | 0.1 |
| (1,276) | 1:50:A:ARG:HB3 | 1:54:A:SER:H | 19 | 0.1 |
| (1,257) | 1:50:A:ARG:H | 1:51:A:ALA:H | 5 | 0.1 |
| (1,257) | 1:50:A:ARG:H | 1:51:A:ALA:H | 20 | 0.1 |
| (1,256) | 1:50:A:ARG:H | 1:51:A:ALA:H | 5 | 0.1 |
| (1,256) | 1:50:A:ARG:H | 1:51:A:ALA:H | 20 | 0.1 |
| (1,192) | 1:36:A:ARG:HG2 | 1:40:A:SER:H | 2 | 0.1 |
| (1,192) | 1:36:A:ARG:HG3 | 1:40:A:SER:H | 2 | 0.1 |
| (1,184) | 1:37:A:THR:H | 1:39:A:VAL:H | 18 | 0.1 |
| (1,101) | 1:27:A:ASN:H | 1:27:A:ASN:HB2 | 10 | 0.1 |
| (1,101) | 1:27:A:ASN:H | 1:27:A:ASN:HB3 | 10 | 0.1 |
| (1,69) | 1:21:A:VAL:HG11 | 1:22:A:ALA:H | 18 | 0.1 |
| (1,69) | 1:21:A:VAL:HG12 | 1:22:A:ALA:H | 18 | 0.1 |
| (1,69) | 1:21:A:VAL:HG13 | 1:22:A:ALA:H | 18 | 0.1 |
| (1,69) | 1:21:A:VAL:HG21 | 1:22:A:ALA:H | 18 | 0.1 |
| (1,69) | 1:21:A:VAL:HG22 | 1:22:A:ALA:H | 18 | 0.1 |
| (1,69) | 1:21:A:VAL:HG23 | 1:22:A:ALA:H | 18 | 0.1 |
| (1,23) | 1:11:A:GLY:HA2 | 1:14:A:SER:H | 3 | 0.1 |
| (1,23) | 1:11:A:GLY:HA3 | 1:14:A:SER:H | 3 | 0.1 |
| (1,6) | 1:6:A:GLY:HA2 | 1:7:A:PHE:H | 8 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|-------|---------------|-------------|----------|---------------|
| (1,6) | 1:6:A:GLY:HA3 | 1:7:A:PHE:H | 8 | 0.1 |

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

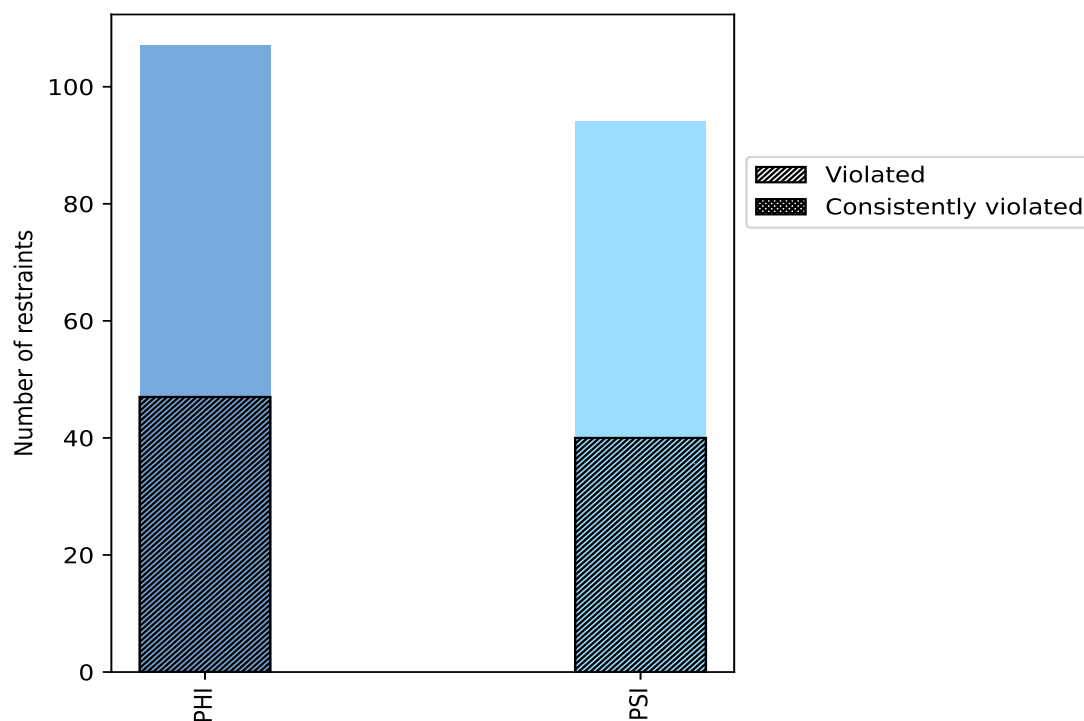
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PHI | 107 | 53.2 | 47 | 43.9 | 23.4 | 0 | 0.0 | 0.0 |
| PSI | 94 | 46.8 | 40 | 42.6 | 19.9 | 0 | 0.0 | 0.0 |
| Total | 201 | 100.0 | 87 | 43.3 | 43.3 | 0 | 0.0 | 0.0 |

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

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



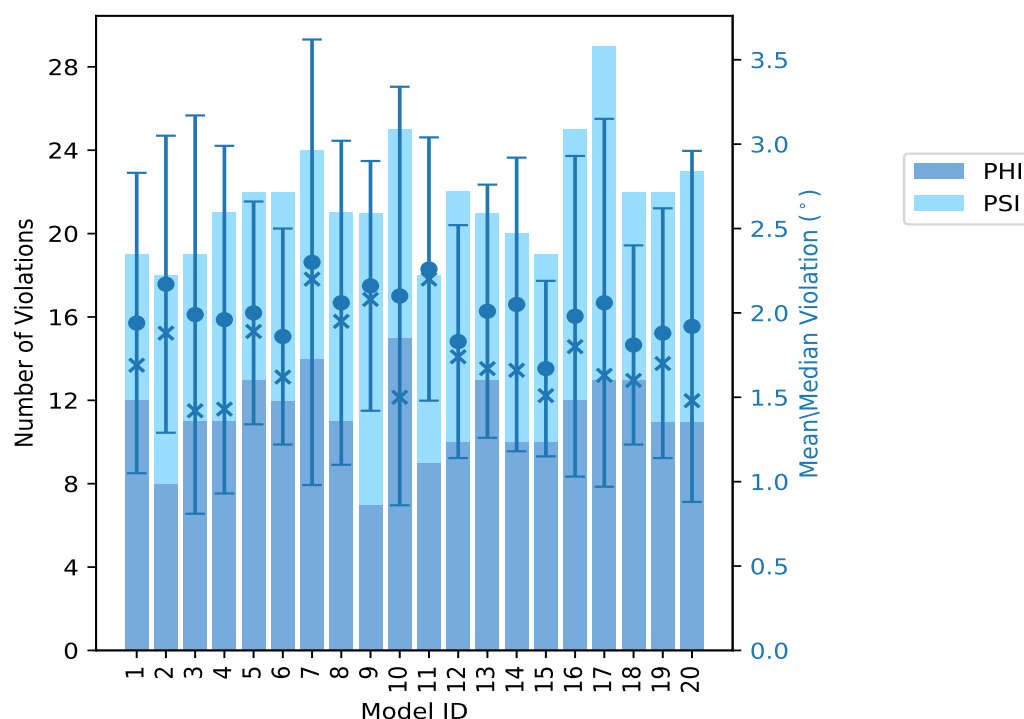
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PHI | PSI | Total | | | | |
| 1 | 12 | 7 | 19 | 1.94 | 4.68 | 0.89 | 1.69 |
| 2 | 8 | 10 | 18 | 2.17 | 4.23 | 0.88 | 1.88 |
| 3 | 11 | 8 | 19 | 1.99 | 4.63 | 1.18 | 1.42 |
| 4 | 11 | 10 | 21 | 1.96 | 4.16 | 1.03 | 1.43 |
| 5 | 13 | 9 | 22 | 2.0 | 3.43 | 0.66 | 1.89 |
| 6 | 12 | 10 | 22 | 1.86 | 3.03 | 0.64 | 1.62 |
| 7 | 14 | 10 | 24 | 2.3 | 7.81 | 1.32 | 2.2 |
| 8 | 11 | 10 | 21 | 2.06 | 4.54 | 0.96 | 1.95 |
| 9 | 7 | 14 | 21 | 2.16 | 3.78 | 0.74 | 2.08 |
| 10 | 15 | 10 | 25 | 2.1 | 6.24 | 1.24 | 1.5 |
| 11 | 9 | 9 | 18 | 2.26 | 3.96 | 0.78 | 2.2 |
| 12 | 10 | 12 | 22 | 1.83 | 3.85 | 0.69 | 1.74 |
| 13 | 13 | 8 | 21 | 2.01 | 3.74 | 0.75 | 1.67 |
| 14 | 10 | 10 | 20 | 2.05 | 3.47 | 0.87 | 1.66 |
| 15 | 10 | 9 | 19 | 1.67 | 2.99 | 0.52 | 1.51 |
| 16 | 12 | 13 | 25 | 1.98 | 5.72 | 0.95 | 1.8 |
| 17 | 13 | 16 | 29 | 2.06 | 5.05 | 1.09 | 1.63 |
| 18 | 13 | 9 | 22 | 1.81 | 3.2 | 0.59 | 1.6 |
| 19 | 11 | 11 | 22 | 1.88 | 3.42 | 0.74 | 1.7 |
| 20 | 11 | 12 | 23 | 1.92 | 5.55 | 1.04 | 1.48 |

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



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

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

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

| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|------|
| PHI | PSI | Total | Count ¹ | % |
| 16 | 9 | 25 | 1 | 5.0 |
| 12 | 2 | 14 | 2 | 10.0 |
| 0 | 7 | 7 | 3 | 15.0 |
| 1 | 3 | 4 | 4 | 20.0 |
| 3 | 5 | 8 | 5 | 25.0 |
| 2 | 3 | 5 | 6 | 30.0 |
| 2 | 2 | 4 | 7 | 35.0 |
| 0 | 2 | 2 | 8 | 40.0 |
| 0 | 0 | 0 | 9 | 45.0 |
| 1 | 3 | 4 | 10 | 50.0 |
| 2 | 1 | 3 | 11 | 55.0 |

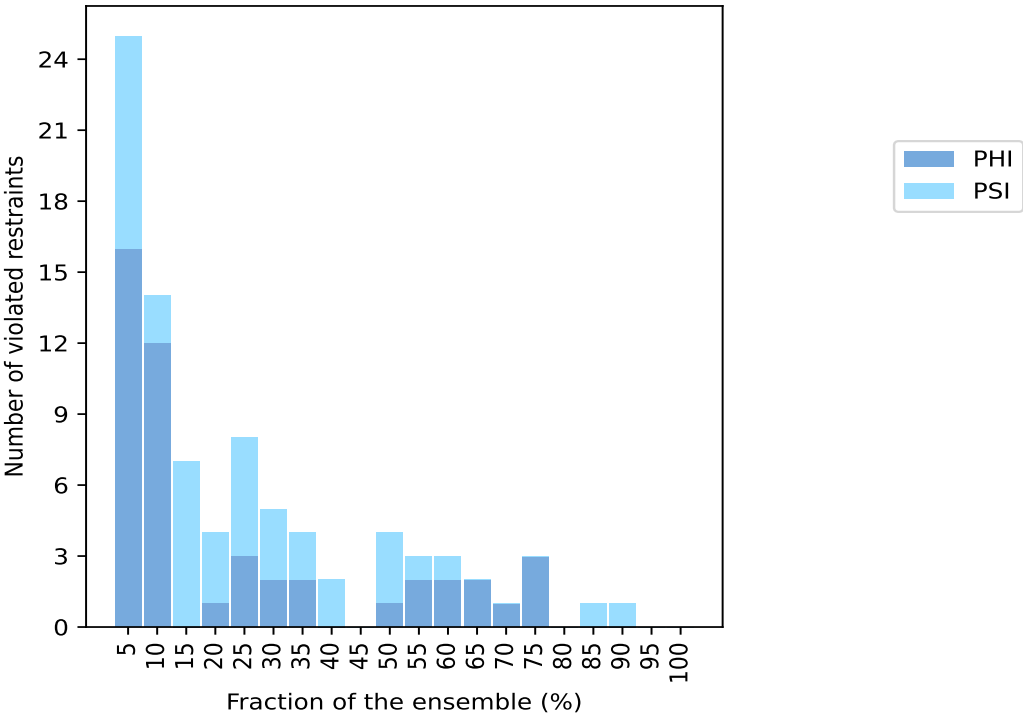
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI | PSI | Total | Count ¹ | % |
| 2 | 1 | 3 | 12 | 60.0 |
| 2 | 0 | 2 | 13 | 65.0 |
| 1 | 0 | 1 | 14 | 70.0 |
| 3 | 0 | 3 | 15 | 75.0 |
| 0 | 0 | 0 | 16 | 80.0 |
| 0 | 1 | 1 | 17 | 85.0 |
| 0 | 1 | 1 | 18 | 90.0 |
| 0 | 0 | 0 | 19 | 95.0 |
| 0 | 0 | 0 | 20 | 100.0 |

¹ Number of models with violations

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

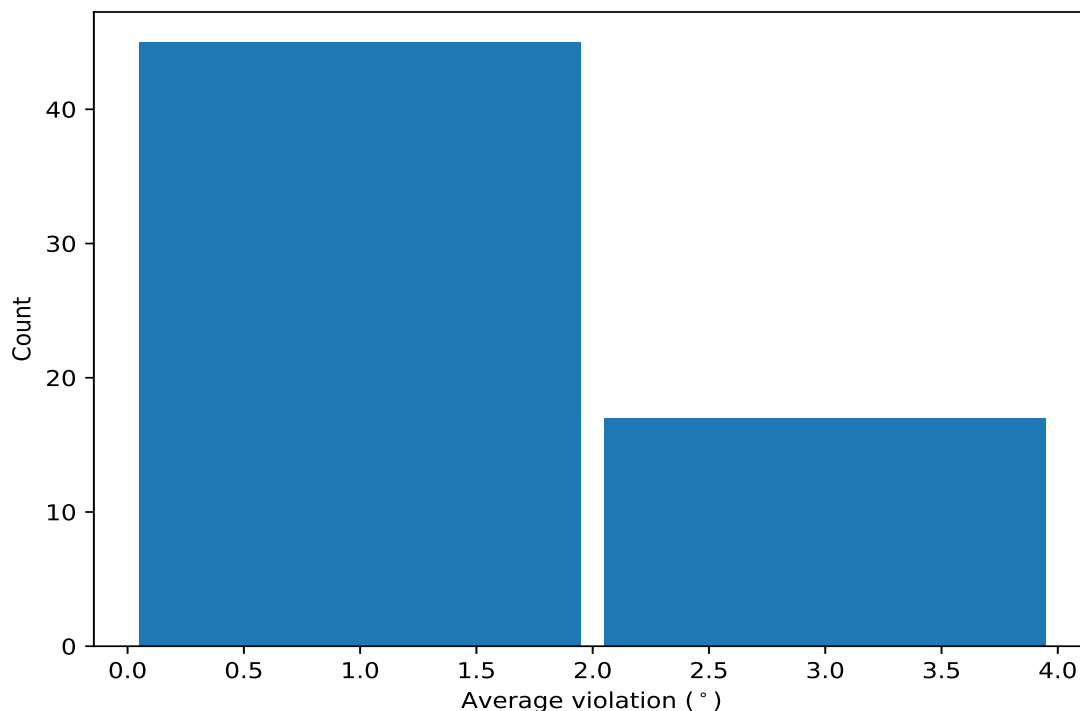


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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 |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 18 | 3.01 | 1.44 | 2.94 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 17 | 2.77 | 0.9 | 2.57 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 15 | 2.43 | 1.1 | 2.36 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 15 | 2.18 | 1.08 | 1.88 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 15 | 1.96 | 0.43 | 1.82 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 14 | 1.9 | 0.6 | 1.78 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 13 | 2.29 | 0.56 | 2.34 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 13 | 2.02 | 0.82 | 2.11 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 12 | 3.25 | 1.41 | 2.96 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 12 | 1.95 | 0.75 | 1.58 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 12 | 1.62 | 0.69 | 1.4 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 11 | 2.29 | 0.39 | 2.3 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 11 | 2.2 | 0.81 | 2.07 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 11 | 1.75 | 0.54 | 1.42 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 10 | 1.96 | 0.94 | 1.51 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 10 | 1.95 | 1.13 | 1.5 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 10 | 1.56 | 0.5 | 1.42 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 10 | 1.46 | 0.29 | 1.44 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 8 | 1.72 | 0.72 | 1.44 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 8 | 1.69 | 0.48 | 1.69 |

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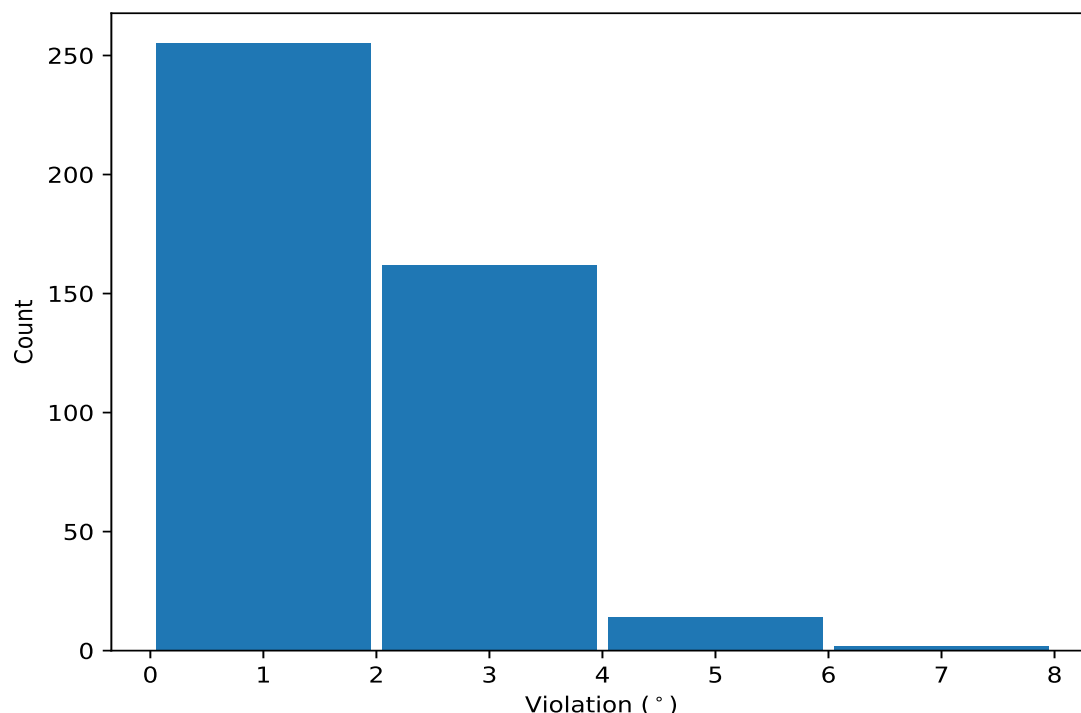
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 7 | 1.98 | 0.95 | 1.78 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 7 | 1.97 | 0.46 | 1.82 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 7 | 1.62 | 0.42 | 1.61 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 7 | 1.51 | 0.75 | 1.19 |
| (1,16) | 1:23:A:ASN:N | 1:23:A:ASN:CA | 1:23:A:ASN:C | 1:24:A:ALA:N | 6 | 2.34 | 0.76 | 2.2 |
| (1,114) | 1:94:A:LEU:C | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 6 | 2.24 | 0.67 | 2.48 |
| (1,102) | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 1:89:A:ALA:N | 6 | 2.1 | 0.92 | 1.92 |
| (1,170) | 1:131:A:VAL:C | 1:132:A:ASP:N | 1:132:A:ASP:CA | 1:132:A:ASP:C | 6 | 1.69 | 0.42 | 1.64 |
| (1,87) | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 1:79:A:ALA:N | 6 | 1.4 | 0.44 | 1.26 |
| (1,197) | 1:147:A:LEU:N | 1:147:A:LEU:CA | 1:147:A:LEU:C | 1:148:A:SER:N | 5 | 3.04 | 1.01 | 3.22 |
| (1,47) | 1:47:A:VAL:N | 1:47:A:VAL:CA | 1:47:A:VAL:C | 1:48:A:VAL:N | 5 | 2.41 | 1.03 | 2.75 |
| (1,157) | 1:121:A:SER:C | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 5 | 1.87 | 0.23 | 1.84 |
| (1,98) | 1:85:A:ALA:N | 1:85:A:ALA:CA | 1:85:A:ALA:C | 1:86:A:TYR:N | 5 | 1.75 | 0.53 | 1.53 |
| (1,137) | 1:110:A:SER:C | 1:111:A:ARG:N | 1:111:A:ARG:CA | 1:111:A:ARG:C | 5 | 1.74 | 0.65 | 1.63 |
| (1,52) | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C | 1:54:A:SER:N | 5 | 1.6 | 0.62 | 1.43 |
| (1,71) | 1:70:A:ALA:N | 1:70:A:ALA:CA | 1:70:A:ALA:C | 1:71:A:VAL:N | 5 | 1.6 | 0.38 | 1.66 |
| (1,49) | 1:48:A:VAL:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 5 | 1.26 | 0.24 | 1.14 |
| (1,8) | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 1:18:A:ILE:N | 4 | 2.35 | 0.64 | 2.22 |
| (1,194) | 1:145:A:SER:C | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 4 | 1.97 | 0.42 | 1.8 |
| (1,12) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:VAL:N | 4 | 1.88 | 0.73 | 1.72 |
| (1,166) | 1:127:A:LEU:N | 1:127:A:LEU:CA | 1:127:A:LEU:C | 1:128:A:GLY:N | 4 | 1.61 | 0.61 | 1.36 |
| (1,195) | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 1:147:A:LEU:N | 3 | 2.27 | 1.39 | 1.48 |
| (1,64) | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 1:62:A:ASP:N | 3 | 2.02 | 0.26 | 2.11 |
| (1,175) | 1:136:A:VAL:N | 1:136:A:VAL:CA | 1:136:A:VAL:C | 1:137:A:GLN:N | 3 | 1.94 | 0.27 | 2.06 |
| (1,55) | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 1:56:A:ALA:N | 3 | 1.73 | 0.39 | 1.59 |
| (1,189) | 1:143:A:SER:N | 1:143:A:SER:CA | 1:143:A:SER:C | 1:144:A:SER:N | 3 | 1.7 | 0.81 | 1.21 |
| (1,60) | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 1:60:A:GLY:N | 3 | 1.34 | 0.18 | 1.29 |
| (1,69) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C | 1:70:A:ALA:N | 3 | 1.2 | 0.22 | 1.06 |
| (1,192) | 1:144:A:SER:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 2 | 1.88 | 0.45 | 1.88 |
| (1,68) | 1:66:A:LEU:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 2 | 1.74 | 0.15 | 1.74 |
| (1,101) | 1:87:A:ALA:C | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 2 | 1.68 | 0.57 | 1.68 |
| (1,62) | 1:60:A:GLY:N | 1:60:A:GLY:CA | 1:60:A:GLY:C | 1:61:A:VAL:N | 2 | 1.64 | 0.28 | 1.64 |
| (1,200) | 1:182:A:TYR:C | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 2 | 1.52 | 0.29 | 1.52 |
| (1,174) | 1:135:A:SER:C | 1:136:A:VAL:N | 1:136:A:VAL:CA | 1:136:A:VAL:C | 2 | 1.42 | 0.24 | 1.42 |
| (1,139) | 1:111:A:ARG:C | 1:112:A:VAL:N | 1:112:A:VAL:CA | 1:112:A:VAL:C | 2 | 1.39 | 0.02 | 1.39 |
| (1,151) | 1:118:A:ASN:C | 1:119:A:GLY:N | 1:119:A:GLY:CA | 1:119:A:GLY:C | 2 | 1.39 | 0.34 | 1.39 |
| (1,113) | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 1:95:A:PHE:N | 2 | 1.33 | 0.27 | 1.33 |
| (1,159) | 1:122:A:SER:C | 1:123:A:ALA:N | 1:123:A:ALA:CA | 1:123:A:ALA:C | 2 | 1.3 | 0.14 | 1.3 |
| (1,110) | 1:92:A:SER:C | 1:93:A:ALA:N | 1:93:A:ALA:CA | 1:93:A:ALA:C | 2 | 1.27 | 0.04 | 1.27 |
| (1,5) | 1:15:A:ALA:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 2 | 1.23 | 0.03 | 1.23 |
| (1,105) | 1:89:A:ALA:C | 1:90:A:PHE:N | 1:90:A:PHE:CA | 1:90:A:PHE:C | 2 | 1.19 | 0.02 | 1.19 |
| (1,164) | 1:125:A:GLN:C | 1:126:A:GLY:N | 1:126:A:GLY:CA | 1:126:A:GLY:C | 2 | 1.14 | 0.03 | 1.14 |

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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 7 | 7.81 |
| (1,100) | 1:86:A:TYR:C | 1:87:A:ALA:N | 1:87:A:ALA:CA | 1:87:A:ALA:C | 10 | 6.24 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 16 | 5.72 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 20 | 5.55 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 17 | 5.05 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 17 | 4.76 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 1 | 4.68 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 3 | 4.63 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 8 | 4.54 |
| (1,197) | 1:147:A:LEU:N | 1:147:A:LEU:CA | 1:147:A:LEU:C | 1:148:A:SER:N | 10 | 4.48 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 3 | 4.34 |
| (1,195) | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 1:147:A:LEU:N | 2 | 4.23 |
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 4 | 4.16 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 8 | 4.05 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 4 | 4.04 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 4 | 4.01 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 11 | 3.96 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 12 | 3.85 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 11 | 3.78 |
| (1,16) | 1:23:A:ASN:N | 1:23:A:ASN:CA | 1:23:A:ASN:C | 1:24:A:ALA:N | 9 | 3.78 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 13 | 3.74 |
| (1,102) | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 1:89:A:ALA:N | 16 | 3.72 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 3 | 3.7 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 3 | 3.7 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 7 | 3.65 |
| (1,47) | 1:47:A:VAL:N | 1:47:A:VAL:CA | 1:47:A:VAL:C | 1:48:A:VAL:N | 9 | 3.61 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 20 | 3.59 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 2 | 3.59 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 17 | 3.54 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 17 | 3.54 |
| (1,197) | 1:147:A:LEU:N | 1:147:A:LEU:CA | 1:147:A:LEU:C | 1:148:A:SER:N | 14 | 3.47 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 5 | 3.43 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 9 | 3.43 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 19 | 3.42 |
| (1,28) | 1:31:A:LEU:C | 1:32:A:ARG:N | 1:32:A:ARG:CA | 1:32:A:ARG:C | 14 | 3.42 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1 | 3.37 |
| (1,8) | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 1:18:A:ILE:N | 10 | 3.34 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 14 | 3.32 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 8 | 3.31 |
| (1,47) | 1:47:A:VAL:N | 1:47:A:VAL:CA | 1:47:A:VAL:C | 1:48:A:VAL:N | 10 | 3.31 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 4 | 3.3 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 14 | 3.26 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 13 | 3.25 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 14 | 3.23 |
| (1,197) | 1:147:A:LEU:N | 1:147:A:LEU:CA | 1:147:A:LEU:C | 1:148:A:SER:N | 5 | 3.22 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 18 | 3.2 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 13 | 3.2 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 18 | 3.19 |
| (1,114) | 1:94:A:LEU:C | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 7 | 3.08 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 6 | 3.03 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 11 | 3.02 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 6 | 3.0 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 10 | 3.0 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 13 | 2.99 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 2 | 2.99 |
| (1,12) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:VAL:N | 15 | 2.99 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 19 | 2.98 |
| (1,137) | 1:110:A:SER:C | 1:111:A:ARG:N | 1:111:A:ARG:CA | 1:111:A:ARG:C | 17 | 2.96 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 9 | 2.92 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 19 | 2.88 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 6 | 2.86 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 19 | 2.85 |
| (1,189) | 1:143:A:SER:N | 1:143:A:SER:CA | 1:143:A:SER:C | 1:144:A:SER:N | 11 | 2.84 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 19 | 2.84 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 2 | 2.8 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 7 | 2.8 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 5 | 2.79 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 13 | 2.79 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 2 | 2.79 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 18 | 2.78 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 15 | 2.77 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 7 | 2.76 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 2 | 2.75 |
| (1,47) | 1:47:A:VAL:N | 1:47:A:VAL:CA | 1:47:A:VAL:C | 1:48:A:VAL:N | 19 | 2.75 |
| (1,52) | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C | 1:54:A:SER:N | 3 | 2.74 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 20 | 2.74 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 11 | 2.73 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 17 | 2.73 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 14 | 2.72 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 10 | 2.7 |
| (1,33) | 1:37:A:THR:N | 1:37:A:THR:CA | 1:37:A:THR:C | 1:38:A:GLY:N | 20 | 2.7 |
| (1,194) | 1:145:A:SER:C | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 17 | 2.68 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 7 | 2.68 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 5 | 2.67 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 6 | 2.66 |
| (1,114) | 1:94:A:LEU:C | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 5 | 2.64 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 17 | 2.64 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 12 | 2.63 |
| (1,166) | 1:127:A:LEU:N | 1:127:A:LEU:CA | 1:127:A:LEU:C | 1:128:A:GLY:N | 14 | 2.63 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 8 | 2.63 |
| (1,114) | 1:94:A:LEU:C | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 17 | 2.62 |
| (1,197) | 1:147:A:LEU:N | 1:147:A:LEU:CA | 1:147:A:LEU:C | 1:148:A:SER:N | 1 | 2.61 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 20 | 2.6 |
| (1,102) | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 1:89:A:ALA:N | 13 | 2.59 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 12 | 2.59 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 1 | 2.59 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 8 | 2.58 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 4 | 2.58 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 9 | 2.58 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 10 | 2.57 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 20 | 2.57 |
| (1,98) | 1:85:A:ALA:N | 1:85:A:ALA:CA | 1:85:A:ALA:C | 1:86:A:TYR:N | 2 | 2.56 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 12 | 2.54 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 2 | 2.53 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 5 | 2.53 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 7 | 2.52 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 10 | 2.52 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 6 | 2.52 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 16 | 2.51 |
| (1,16) | 1:23:A:ASN:N | 1:23:A:ASN:CA | 1:23:A:ASN:C | 1:24:A:ALA:N | 17 | 2.51 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 17 | 2.5 |
| (1,102) | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 1:89:A:ALA:N | 4 | 2.46 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 10 | 2.46 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 8 | 2.46 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 9 | 2.46 |
| (1,8) | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 1:18:A:ILE:N | 16 | 2.45 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 9 | 2.44 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 20 | 2.43 |
| (1,186) | 1:141:A:SER:C | 1:142:A:SER:N | 1:142:A:SER:CA | 1:142:A:SER:C | 11 | 2.42 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 18 | 2.38 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 13 | 2.36 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 11 | 2.36 |
| (1,170) | 1:131:A:VAL:C | 1:132:A:ASP:N | 1:132:A:ASP:CA | 1:132:A:ASP:C | 1 | 2.35 |
| (1,87) | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 1:79:A:ALA:N | 7 | 2.34 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 10 | 2.34 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 8 | 2.34 |
| (1,192) | 1:144:A:SER:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 7 | 2.33 |
| (1,114) | 1:94:A:LEU:C | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 6 | 2.33 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 5 | 2.32 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 14 | 2.31 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 8 | 2.3 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 12 | 2.3 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 7 | 2.29 |
| (1,64) | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 1:62:A:ASP:N | 7 | 2.29 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 1 | 2.28 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 11 | 2.28 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 7 | 2.27 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 16 | 2.27 |
| (1,55) | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 1:56:A:ALA:N | 15 | 2.26 |
| (1,101) | 1:87:A:ALA:C | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 16 | 2.25 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 6 | 2.23 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 18 | 2.23 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 19 | 2.22 |
| (1,16) | 1:23:A:ASN:N | 1:23:A:ASN:CA | 1:23:A:ASN:C | 1:24:A:ALA:N | 5 | 2.21 |
| (1,175) | 1:136:A:VAL:N | 1:136:A:VAL:CA | 1:136:A:VAL:C | 1:137:A:GLN:N | 16 | 2.2 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 5 | 2.2 |
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 12 | 2.2 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 11 | 2.2 |
| (1,16) | 1:23:A:ASN:N | 1:23:A:ASN:CA | 1:23:A:ASN:C | 1:24:A:ALA:N | 11 | 2.2 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 9 | 2.19 |
| (1,157) | 1:121:A:SER:C | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 1 | 2.18 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 9 | 2.18 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 12 | 2.17 |
| (1,98) | 1:85:A:ALA:N | 1:85:A:ALA:CA | 1:85:A:ALA:C | 1:86:A:TYR:N | 9 | 2.17 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 16 | 2.17 |
| (1,16) | 1:23:A:ASN:N | 1:23:A:ASN:CA | 1:23:A:ASN:C | 1:24:A:ALA:N | 6 | 2.17 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 5 | 2.14 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 7 | 2.12 |
| (1,64) | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 1:62:A:ASP:N | 8 | 2.11 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 3 | 2.11 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 16 | 2.09 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 9 | 2.08 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 6 | 2.08 |
| (1,157) | 1:121:A:SER:C | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 11 | 2.07 |
| (1,71) | 1:70:A:ALA:N | 1:70:A:ALA:CA | 1:70:A:ALA:C | 1:71:A:VAL:N | 18 | 2.07 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 20 | 2.07 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 11 | 2.07 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,12) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:VAL:N | 17 | 2.07 |
| (1,175) | 1:136:A:VAL:N | 1:136:A:VAL:CA | 1:136:A:VAL:C | 1:137:A:GLN:N | 12 | 2.06 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 15 | 2.06 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 7 | 2.06 |
| (1,118) | 1:98:A:GLY:N | 1:98:A:GLY:CA | 1:98:A:GLY:C | 1:99:A:VAL:N | 12 | 2.05 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 16 | 2.05 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 17 | 2.02 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 12 | 2.02 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 2 | 2.01 |
| (1,170) | 1:131:A:VAL:C | 1:132:A:ASP:N | 1:132:A:ASP:CA | 1:132:A:ASP:C | 10 | 2.0 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 4 | 2.0 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 16 | 1.98 |
| (1,8) | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 1:18:A:ILE:N | 8 | 1.98 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 12 | 1.96 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 5 | 1.96 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 8 | 1.95 |
| (1,71) | 1:70:A:ALA:N | 1:70:A:ALA:CA | 1:70:A:ALA:C | 1:71:A:VAL:N | 19 | 1.92 |
| (1,62) | 1:60:A:GLY:N | 1:60:A:GLY:CA | 1:60:A:GLY:C | 1:61:A:VAL:N | 19 | 1.92 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 8 | 1.92 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 4 | 1.91 |
| (1,88) | 1:78:A:PRO:C | 1:79:A:ALA:N | 1:79:A:ALA:CA | 1:79:A:ALA:C | 7 | 1.89 |
| (1,68) | 1:66:A:LEU:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 8 | 1.89 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 20 | 1.88 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 15 | 1.88 |
| (1,194) | 1:145:A:SER:C | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 18 | 1.87 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 19 | 1.87 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 13 | 1.87 |
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 15 | 1.86 |
| (1,157) | 1:121:A:SER:C | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 13 | 1.84 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 11 | 1.84 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 6 | 1.84 |
| (1,170) | 1:131:A:VAL:C | 1:132:A:ASP:N | 1:132:A:ASP:CA | 1:132:A:ASP:C | 4 | 1.83 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 15 | 1.83 |
| (1,86) | 1:77:A:LEU:C | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 13 | 1.82 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 5 | 1.82 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 9 | 1.82 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 7 | 1.82 |
| (1,200) | 1:182:A:TYR:C | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 16 | 1.8 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 16 | 1.8 |
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 18 | 1.78 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 5 | 1.78 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 3 | 1.77 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 2 | 1.75 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 1 | 1.74 |
| (1,151) | 1:118:A:ASN:C | 1:119:A:GLY:N | 1:119:A:GLY:CA | 1:119:A:GLY:C | 18 | 1.73 |
| (1,194) | 1:145:A:SER:C | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 15 | 1.72 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 14 | 1.72 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 1 | 1.72 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 10 | 1.72 |
| (1,49) | 1:48:A:VAL:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 19 | 1.72 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 2 | 1.71 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 2 | 1.7 |
| (1,52) | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C | 1:54:A:SER:N | 9 | 1.7 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 18 | 1.69 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 1 | 1.69 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 20 | 1.69 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 19 | 1.68 |
| (1,157) | 1:121:A:SER:C | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 7 | 1.67 |
| (1,114) | 1:94:A:LEU:C | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 16 | 1.67 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 13 | 1.67 |
| (1,64) | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 1:62:A:ASP:N | 14 | 1.67 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 9 | 1.67 |
| (1,174) | 1:135:A:SER:C | 1:136:A:VAL:N | 1:136:A:VAL:CA | 1:136:A:VAL:C | 16 | 1.66 |
| (1,173) | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 1:136:A:VAL:N | 17 | 1.66 |
| (1,71) | 1:70:A:ALA:N | 1:70:A:ALA:CA | 1:70:A:ALA:C | 1:71:A:VAL:N | 14 | 1.66 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 9 | 1.66 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 3 | 1.66 |
| (1,137) | 1:110:A:SER:C | 1:111:A:ARG:N | 1:111:A:ARG:CA | 1:111:A:ARG:C | 9 | 1.64 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 11 | 1.64 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 13 | 1.63 |
| (1,137) | 1:110:A:SER:C | 1:111:A:ARG:N | 1:111:A:ARG:CA | 1:111:A:ARG:C | 1 | 1.63 |
| (1,8) | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 1:18:A:ILE:N | 6 | 1.63 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 11 | 1.63 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 17 | 1.63 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 18 | 1.62 |
| (1,194) | 1:145:A:SER:C | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 6 | 1.61 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 7 | 1.61 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 6 | 1.61 |
| (1,113) | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 1:95:A:PHE:N | 5 | 1.6 |
| (1,157) | 1:121:A:SER:C | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 16 | 1.59 |
| (1,68) | 1:66:A:LEU:C | 1:67:A:ALA:N | 1:67:A:ALA:CA | 1:67:A:ALA:C | 9 | 1.59 |
| (1,60) | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 1:60:A:GLY:N | 18 | 1.59 |
| (1,55) | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 1:56:A:ALA:N | 14 | 1.59 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 14 | 1.59 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 20 | 1.58 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 4 | 1.58 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 16 | 1.58 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 19 | 1.57 |
| (1,175) | 1:136:A:VAL:N | 1:136:A:VAL:CA | 1:136:A:VAL:C | 1:137:A:GLN:N | 13 | 1.57 |
| (1,188) | 1:142:A:SER:C | 1:143:A:SER:N | 1:143:A:SER:CA | 1:143:A:SER:C | 9 | 1.56 |
| (1,82) | 1:75:A:SER:C | 1:76:A:ARG:N | 1:76:A:ARG:CA | 1:76:A:ARG:C | 9 | 1.55 |
| (1,45) | 1:45:A:SER:N | 1:45:A:SER:CA | 1:45:A:SER:C | 1:46:A:SER:N | 6 | 1.55 |
| (1,98) | 1:85:A:ALA:N | 1:85:A:ALA:CA | 1:85:A:ALA:C | 1:86:A:TYR:N | 15 | 1.53 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 18 | 1.53 |
| (1,103) | 1:88:A:GLN:C | 1:89:A:ALA:N | 1:89:A:ALA:CA | 1:89:A:ALA:C | 16 | 1.52 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 5 | 1.52 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 6 | 1.52 |
| (1,166) | 1:127:A:LEU:N | 1:127:A:LEU:CA | 1:127:A:LEU:C | 1:128:A:GLY:N | 18 | 1.51 |
| (1,69) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C | 1:70:A:ALA:N | 12 | 1.51 |
| (1,48) | 1:47:A:VAL:C | 1:48:A:VAL:N | 1:48:A:VAL:CA | 1:48:A:VAL:C | 15 | 1.51 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 13 | 1.51 |
| (1,107) | 1:91:A:SER:N | 1:91:A:SER:CA | 1:91:A:SER:C | 1:92:A:SER:N | 10 | 1.5 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 12 | 1.49 |
| (1,195) | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 1:147:A:LEU:N | 20 | 1.48 |
| (1,119) | 1:98:A:GLY:C | 1:99:A:VAL:N | 1:99:A:VAL:CA | 1:99:A:VAL:C | 17 | 1.48 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 8 | 1.48 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 5 | 1.47 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 10 | 1.46 |
| (1,170) | 1:131:A:VAL:C | 1:132:A:ASP:N | 1:132:A:ASP:CA | 1:132:A:ASP:C | 13 | 1.45 |
| (1,137) | 1:110:A:SER:C | 1:111:A:ARG:N | 1:111:A:ARG:CA | 1:111:A:ARG:C | 3 | 1.45 |
| (1,87) | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 1:79:A:ALA:N | 2 | 1.45 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 15 | 1.45 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 2 | 1.45 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 14 | 1.45 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 18 | 1.44 |
| (1,192) | 1:144:A:SER:C | 1:145:A:SER:N | 1:145:A:SER:CA | 1:145:A:SER:C | 13 | 1.43 |
| (1,159) | 1:122:A:SER:C | 1:123:A:ALA:N | 1:123:A:ALA:CA | 1:123:A:ALA:C | 18 | 1.43 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 4 | 1.43 |
| (1,94) | 1:83:A:THR:N | 1:83:A:THR:CA | 1:83:A:THR:C | 1:84:A:SER:N | 7 | 1.43 |
| (1,52) | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C | 1:54:A:SER:N | 18 | 1.43 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 20 | 1.43 |
| (1,170) | 1:131:A:VAL:C | 1:132:A:ASP:N | 1:132:A:ASP:CA | 1:132:A:ASP:C | 3 | 1.42 |
| (1,156) | 1:121:A:SER:N | 1:121:A:SER:CA | 1:121:A:SER:C | 1:122:A:SER:N | 20 | 1.42 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 13 | 1.42 |
| (1,197) | 1:147:A:LEU:N | 1:147:A:LEU:CA | 1:147:A:LEU:C | 1:148:A:SER:N | 19 | 1.41 |
| (1,139) | 1:111:A:ARG:C | 1:112:A:VAL:N | 1:112:A:VAL:CA | 1:112:A:VAL:C | 16 | 1.41 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 2 | 1.41 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 1 | 1.41 |
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 5 | 1.4 |
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 10 | 1.4 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 12 | 1.4 |
| (1,27) | 1:31:A:LEU:N | 1:31:A:LEU:CA | 1:31:A:LEU:C | 1:32:A:ARG:N | 15 | 1.4 |
| (1,102) | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 1:89:A:ALA:N | 12 | 1.39 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 1 | 1.39 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 6 | 1.38 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 4 | 1.38 |
| (1,139) | 1:111:A:ARG:C | 1:112:A:VAL:N | 1:112:A:VAL:CA | 1:112:A:VAL:C | 18 | 1.37 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 19 | 1.37 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 3 | 1.37 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 17 | 1.37 |
| (1,12) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:VAL:N | 18 | 1.37 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 13 | 1.37 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 15 | 1.36 |
| (1,62) | 1:60:A:GLY:N | 1:60:A:GLY:CA | 1:60:A:GLY:C | 1:61:A:VAL:N | 4 | 1.35 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 13 | 1.35 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 10 | 1.34 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 5 | 1.33 |
| (1,67) | 1:65:A:ASN:C | 1:66:A:LEU:N | 1:66:A:LEU:CA | 1:66:A:LEU:C | 17 | 1.33 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 17 | 1.33 |
| (1,55) | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 1:56:A:ALA:N | 16 | 1.33 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 13 | 1.32 |
| (1,24) | 1:29:A:SER:N | 1:29:A:SER:CA | 1:29:A:SER:C | 1:30:A:THR:N | 10 | 1.32 |
| (1,110) | 1:92:A:SER:C | 1:93:A:ALA:N | 1:93:A:ALA:CA | 1:93:A:ALA:C | 6 | 1.31 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,71) | 1:70:A:ALA:N | 1:70:A:ALA:CA | 1:70:A:ALA:C | 1:71:A:VAL:N | 12 | 1.31 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 1 | 1.3 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 1 | 1.3 |
| (1,46) | 1:45:A:SER:C | 1:46:A:SER:N | 1:46:A:SER:CA | 1:46:A:SER:C | 5 | 1.3 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 20 | 1.3 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 3 | 1.29 |
| (1,102) | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 1:89:A:ALA:N | 15 | 1.29 |
| (1,60) | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 1:60:A:GLY:N | 17 | 1.29 |
| (1,34) | 1:37:A:THR:C | 1:38:A:GLY:N | 1:38:A:GLY:CA | 1:38:A:GLY:C | 19 | 1.29 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 5 | 1.29 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 5 | 1.27 |
| (1,87) | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 1:79:A:ALA:N | 1 | 1.26 |
| (1,87) | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 1:79:A:ALA:N | 11 | 1.26 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 11 | 1.26 |
| (1,56) | 1:55:A:LEU:C | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 4 | 1.26 |
| (1,49) | 1:48:A:VAL:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 14 | 1.26 |
| (1,47) | 1:47:A:VAL:N | 1:47:A:VAL:CA | 1:47:A:VAL:C | 1:48:A:VAL:N | 16 | 1.26 |
| (1,5) | 1:15:A:ALA:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 6 | 1.26 |
| (1,153) | 1:119:A:GLY:C | 1:120:A:VAL:N | 1:120:A:VAL:CA | 1:120:A:VAL:C | 20 | 1.25 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 15 | 1.25 |
| (1,54) | 1:54:A:SER:C | 1:55:A:LEU:N | 1:55:A:LEU:CA | 1:55:A:LEU:C | 4 | 1.25 |
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 20 | 1.24 |
| (1,110) | 1:92:A:SER:C | 1:93:A:ALA:N | 1:93:A:ALA:CA | 1:93:A:ALA:C | 8 | 1.24 |
| (1,98) | 1:85:A:ALA:N | 1:85:A:ALA:CA | 1:85:A:ALA:C | 1:86:A:TYR:N | 19 | 1.24 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 7 | 1.24 |
| (1,200) | 1:182:A:TYR:C | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 17 | 1.23 |
| (1,98) | 1:85:A:ALA:N | 1:85:A:ALA:CA | 1:85:A:ALA:C | 1:86:A:TYR:N | 16 | 1.23 |
| (1,166) | 1:127:A:LEU:N | 1:127:A:LEU:CA | 1:127:A:LEU:C | 1:128:A:GLY:N | 4 | 1.22 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 9 | 1.22 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 18 | 1.22 |
| (1,189) | 1:143:A:SER:N | 1:143:A:SER:CA | 1:143:A:SER:C | 1:144:A:SER:N | 20 | 1.21 |
| (1,105) | 1:89:A:ALA:C | 1:90:A:PHE:N | 1:90:A:PHE:CA | 1:90:A:PHE:C | 18 | 1.21 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 15 | 1.21 |
| (1,5) | 1:15:A:ALA:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 10 | 1.21 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 7 | 1.2 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 1 | 1.2 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 19 | 1.2 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 8 | 1.19 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 14 | 1.19 |
| (1,16) | 1:23:A:ASN:N | 1:23:A:ASN:CA | 1:23:A:ASN:C | 1:24:A:ALA:N | 7 | 1.19 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 12 | 1.19 |
| (1,174) | 1:135:A:SER:C | 1:136:A:VAL:N | 1:136:A:VAL:CA | 1:136:A:VAL:C | 12 | 1.18 |
| (1,164) | 1:125:A:GLN:C | 1:126:A:GLY:N | 1:126:A:GLY:CA | 1:126:A:GLY:C | 15 | 1.18 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 18 | 1.17 |
| (1,105) | 1:89:A:ALA:C | 1:90:A:PHE:N | 1:90:A:PHE:CA | 1:90:A:PHE:C | 10 | 1.17 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 12 | 1.17 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 1 | 1.17 |
| (1,159) | 1:122:A:SER:C | 1:123:A:ALA:N | 1:123:A:ALA:CA | 1:123:A:ALA:C | 15 | 1.16 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 10 | 1.16 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 14 | 1.15 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 16 | 1.15 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 4 | 1.15 |
| (1,60) | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 1:60:A:GLY:N | 14 | 1.15 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 3 | 1.15 |
| (1,49) | 1:48:A:VAL:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 4 | 1.14 |
| (1,96) | 1:84:A:SER:N | 1:84:A:SER:CA | 1:84:A:SER:C | 1:85:A:ALA:N | 6 | 1.13 |
| (1,47) | 1:47:A:VAL:N | 1:47:A:VAL:CA | 1:47:A:VAL:C | 1:48:A:VAL:N | 17 | 1.13 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 2 | 1.13 |
| (1,102) | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 1:89:A:ALA:N | 3 | 1.12 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 4 | 1.12 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 8 | 1.12 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 6 | 1.12 |
| (1,199) | 1:148:A:SER:N | 1:148:A:SER:CA | 1:148:A:SER:C | 1:149:A:THR:N | 7 | 1.11 |
| (1,164) | 1:125:A:GLN:C | 1:126:A:GLY:N | 1:126:A:GLY:CA | 1:126:A:GLY:C | 3 | 1.11 |
| (1,112) | 1:93:A:ALA:C | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 17 | 1.11 |
| (1,52) | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C | 1:54:A:SER:N | 17 | 1.11 |
| (1,49) | 1:48:A:VAL:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 15 | 1.11 |
| (1,42) | 1:42:A:GLN:C | 1:43:A:ILE:N | 1:43:A:ILE:CA | 1:43:A:ILE:C | 16 | 1.11 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 14 | 1.11 |
| (1,195) | 1:146:A:PHE:N | 1:146:A:PHE:CA | 1:146:A:PHE:C | 1:147:A:LEU:N | 12 | 1.1 |
| (1,101) | 1:87:A:ALA:C | 1:88:A:GLN:N | 1:88:A:GLN:CA | 1:88:A:GLN:C | 8 | 1.1 |
| (1,59) | 1:58:A:THR:C | 1:59:A:LEU:N | 1:59:A:LEU:CA | 1:59:A:LEU:C | 20 | 1.1 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 17 | 1.1 |
| (1,120) | 1:99:A:VAL:C | 1:100:A:LEU:N | 1:100:A:LEU:CA | 1:100:A:LEU:C | 7 | 1.09 |
| (1,49) | 1:48:A:VAL:C | 1:49:A:GLN:N | 1:49:A:GLN:CA | 1:49:A:GLN:C | 3 | 1.09 |
| (1,12) | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 1:21:A:VAL:N | 2 | 1.09 |
| (1,11) | 1:19:A:SER:C | 1:20:A:ARG:N | 1:20:A:ARG:CA | 1:20:A:ARG:C | 10 | 1.09 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 9 | 1.08 |
| (1,170) | 1:131:A:VAL:C | 1:132:A:ASP:N | 1:132:A:ASP:CA | 1:132:A:ASP:C | 12 | 1.08 |
| (1,166) | 1:127:A:LEU:N | 1:127:A:LEU:CA | 1:127:A:LEU:C | 1:128:A:GLY:N | 3 | 1.08 |
| (1,158) | 1:122:A:SER:N | 1:122:A:SER:CA | 1:122:A:SER:C | 1:123:A:ALA:N | 19 | 1.08 |
| (1,114) | 1:94:A:LEU:C | 1:95:A:PHE:N | 1:95:A:PHE:CA | 1:95:A:PHE:C | 20 | 1.08 |
| (1,87) | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 1:79:A:ALA:N | 17 | 1.08 |
| (1,66) | 1:64:A:ASN:C | 1:65:A:ASN:N | 1:65:A:ASN:CA | 1:65:A:ASN:C | 13 | 1.08 |
| (1,63) | 1:60:A:GLY:C | 1:61:A:VAL:N | 1:61:A:VAL:CA | 1:61:A:VAL:C | 6 | 1.08 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 8 | 1.08 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 19 | 1.08 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 10 | 1.08 |
| (1,13) | 1:21:A:VAL:C | 1:22:A:ALA:N | 1:22:A:ALA:CA | 1:22:A:ALA:C | 8 | 1.07 |
| (1,113) | 1:94:A:LEU:N | 1:94:A:LEU:CA | 1:94:A:LEU:C | 1:95:A:PHE:N | 20 | 1.06 |
| (1,76) | 1:72:A:GLN:C | 1:73:A:ALA:N | 1:73:A:ALA:CA | 1:73:A:ALA:C | 5 | 1.06 |
| (1,69) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C | 1:70:A:ALA:N | 17 | 1.06 |
| (1,44) | 1:43:A:ILE:C | 1:44:A:ALA:N | 1:44:A:ALA:CA | 1:44:A:ALA:C | 2 | 1.06 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 20 | 1.06 |
| (1,151) | 1:118:A:ASN:C | 1:119:A:GLY:N | 1:119:A:GLY:CA | 1:119:A:GLY:C | 19 | 1.05 |
| (1,140) | 1:112:A:VAL:N | 1:112:A:VAL:CA | 1:112:A:VAL:C | 1:113:A:LEU:N | 17 | 1.05 |
| (1,39) | 1:41:A:GLN:N | 1:41:A:GLN:CA | 1:41:A:GLN:C | 1:42:A:GLN:N | 20 | 1.05 |
| (1,191) | 1:144:A:SER:N | 1:144:A:SER:CA | 1:144:A:SER:C | 1:145:A:SER:N | 17 | 1.04 |
| (1,189) | 1:143:A:SER:N | 1:143:A:SER:CA | 1:143:A:SER:C | 1:144:A:SER:N | 4 | 1.04 |
| (1,137) | 1:110:A:SER:C | 1:111:A:ARG:N | 1:111:A:ARG:CA | 1:111:A:ARG:C | 14 | 1.04 |
| (1,71) | 1:70:A:ALA:N | 1:70:A:ALA:CA | 1:70:A:ALA:C | 1:71:A:VAL:N | 6 | 1.04 |
| (1,22) | 1:27:A:ASN:N | 1:27:A:ASN:CA | 1:27:A:ASN:C | 1:28:A:THR:N | 4 | 1.04 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,172) | 1:134:A:GLY:C | 1:135:A:SER:N | 1:135:A:SER:CA | 1:135:A:SER:C | 10 | 1.03 |
| (1,171) | 1:132:A:ASP:C | 1:133:A:SER:N | 1:133:A:SER:CA | 1:133:A:SER:C | 11 | 1.03 |
| (1,87) | 1:78:A:PRO:N | 1:78:A:PRO:CA | 1:78:A:PRO:C | 1:79:A:ALA:N | 3 | 1.03 |
| (1,52) | 1:53:A:GLN:N | 1:53:A:GLN:CA | 1:53:A:GLN:C | 1:54:A:SER:N | 10 | 1.03 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 16 | 1.02 |
| (1,69) | 1:69:A:PHE:N | 1:69:A:PHE:CA | 1:69:A:PHE:C | 1:70:A:ALA:N | 10 | 1.02 |
| (1,201) | 1:183:A:PRO:N | 1:183:A:PRO:CA | 1:183:A:PRO:C | 1:184:A:GLY:N | 3 | 1.01 |
| (1,92) | 1:81:A:SER:N | 1:81:A:SER:CA | 1:81:A:SER:C | 1:82:A:ASP:N | 19 | 1.01 |
| (1,57) | 1:56:A:ALA:N | 1:56:A:ALA:CA | 1:56:A:ALA:C | 1:57:A:SER:N | 1 | 1.01 |
| (1,10) | 1:19:A:SER:N | 1:19:A:SER:CA | 1:19:A:SER:C | 1:20:A:ARG:N | 8 | 1.01 |
| (1,7) | 1:16:A:GLY:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 12 | 1.01 |