



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 03:43 PM EST

PDB ID : 2LGO
BMRB ID : 17818
Title : Solution NMR structure of a FKBP-type peptidyl-prolyl cis-trans isomerase from *Giardia lamblia*, Seattle Structural Genomics Center for Infectious Disease target GilaA.00840.a
Authors : Buchko, G.W.; Seattle Structural Genomics Center for Infectious Disease (SS-GCID)
Deposited on : 2011-07-29

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

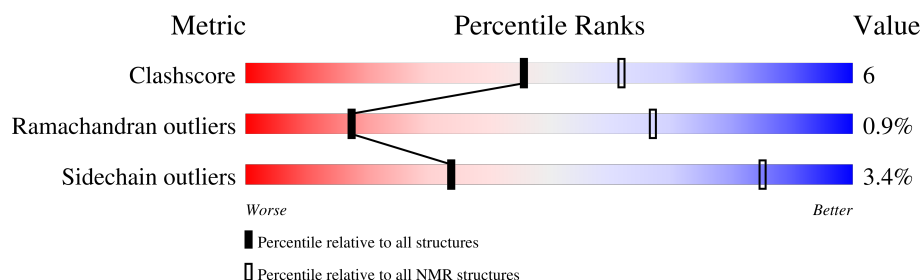
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

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 | 130 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:25-A:130 (106) | 0.92 | 14 |

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1996 atoms, of which 998 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FKBP.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1 | A | 130 | Total | C | H | N | O | S | 0 |
| | | | 1996 | 637 | 998 | 175 | 182 | 4 | |

There are 21 discrepancies between the modelled and reference sequences:

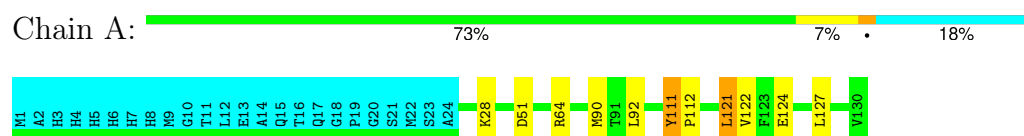
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1 | MET | - | expression tag | UNP Q8I6M8 |
| A | 2 | ALA | - | expression tag | UNP Q8I6M8 |
| A | 3 | HIS | - | expression tag | UNP Q8I6M8 |
| A | 4 | HIS | - | expression tag | UNP Q8I6M8 |
| A | 5 | HIS | - | expression tag | UNP Q8I6M8 |
| A | 6 | HIS | - | expression tag | UNP Q8I6M8 |
| A | 7 | HIS | - | expression tag | UNP Q8I6M8 |
| A | 8 | HIS | - | expression tag | UNP Q8I6M8 |
| A | 9 | MET | - | expression tag | UNP Q8I6M8 |
| A | 10 | GLY | - | expression tag | UNP Q8I6M8 |
| A | 11 | THR | - | expression tag | UNP Q8I6M8 |
| A | 12 | LEU | - | expression tag | UNP Q8I6M8 |
| A | 13 | GLU | - | expression tag | UNP Q8I6M8 |
| A | 14 | ALA | - | expression tag | UNP Q8I6M8 |
| A | 15 | GLN | - | expression tag | UNP Q8I6M8 |
| A | 16 | THR | - | expression tag | UNP Q8I6M8 |
| A | 17 | GLN | - | expression tag | UNP Q8I6M8 |
| A | 18 | GLY | - | expression tag | UNP Q8I6M8 |
| A | 19 | PRO | - | expression tag | UNP Q8I6M8 |
| A | 20 | GLY | - | expression tag | UNP Q8I6M8 |
| A | 21 | SER | - | expression tag | UNP Q8I6M8 |

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: FKBP

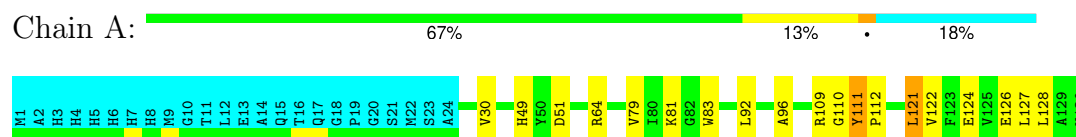


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

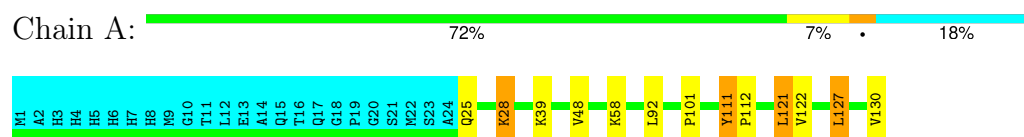
4.2.1 Score per residue for model 1

- Molecule 1: FKBP



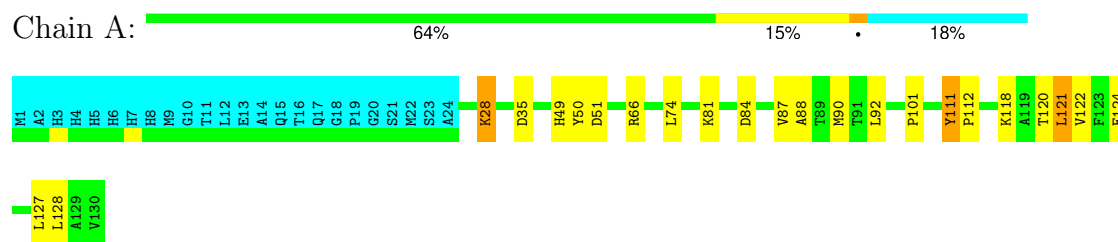
4.2.2 Score per residue for model 2

- Molecule 1: FKBP



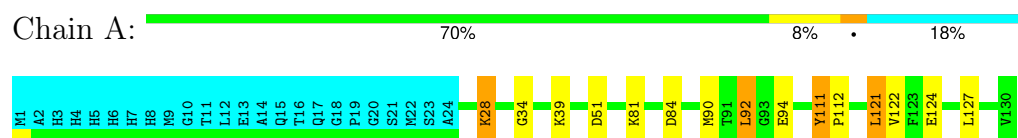
4.2.3 Score per residue for model 3

- Molecule 1: FKBP



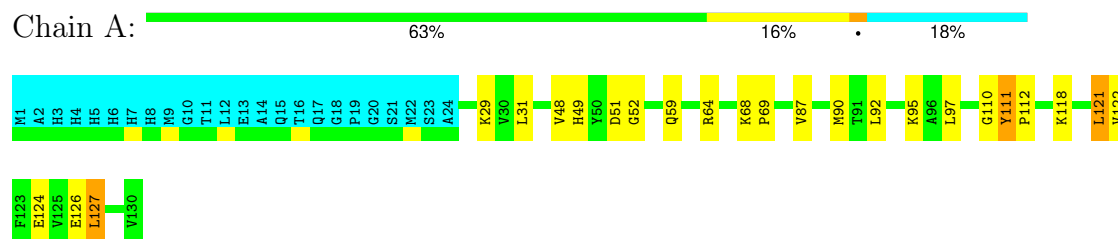
4.2.4 Score per residue for model 4

- Molecule 1: FKBP



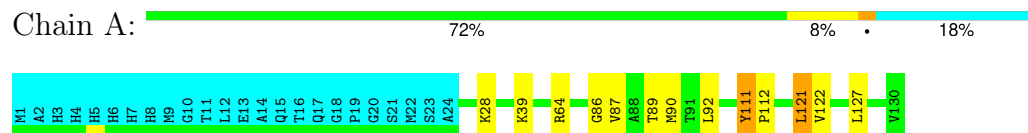
4.2.5 Score per residue for model 5

- Molecule 1: FKBP



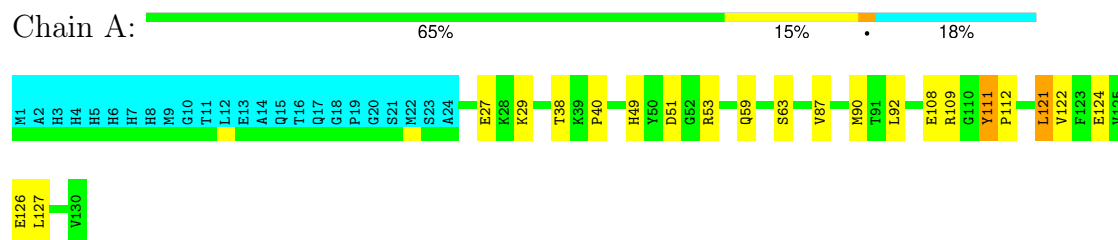
4.2.6 Score per residue for model 6

- Molecule 1: FKBP



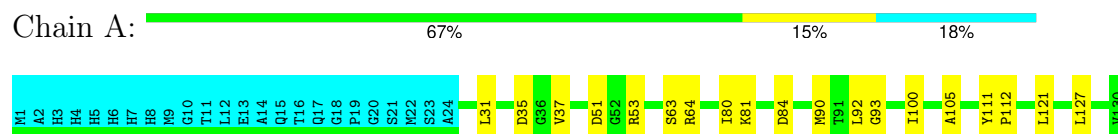
4.2.7 Score per residue for model 7

- Molecule 1: FKBP



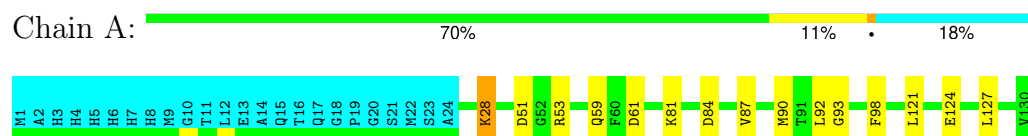
4.2.8 Score per residue for model 8

- Molecule 1: FKBP



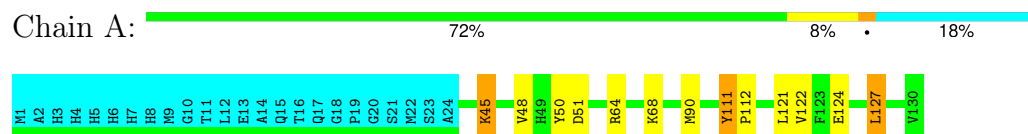
4.2.9 Score per residue for model 9

- Molecule 1: FKBP



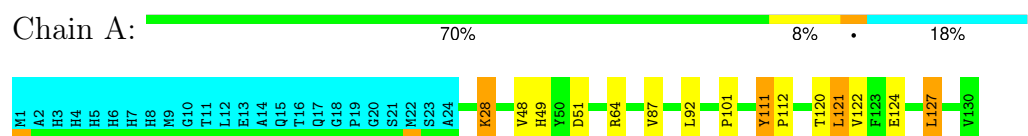
4.2.10 Score per residue for model 10

- Molecule 1: FKBP



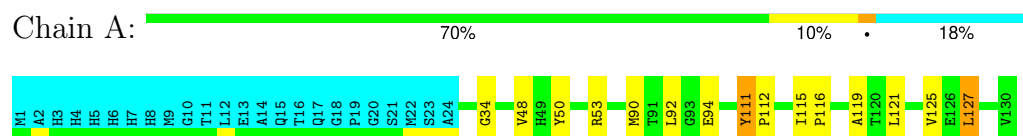
4.2.11 Score per residue for model 11

- Molecule 1: FKBP



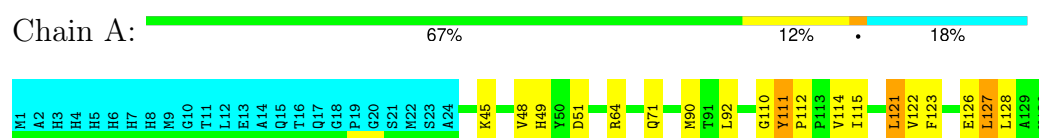
4.2.12 Score per residue for model 12

- Molecule 1: FKBP



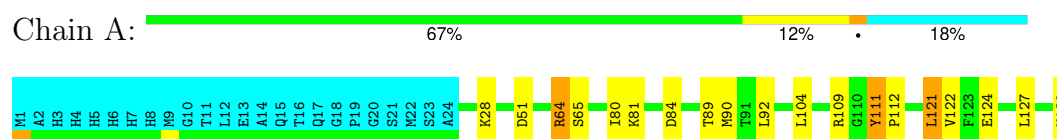
4.2.13 Score per residue for model 13

- Molecule 1: FKBP



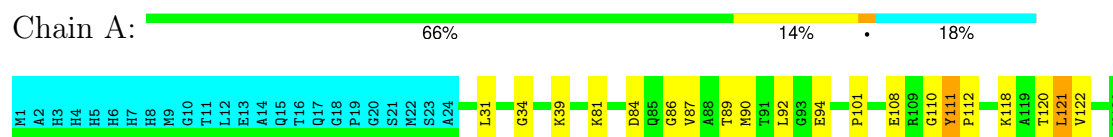
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: FKBP



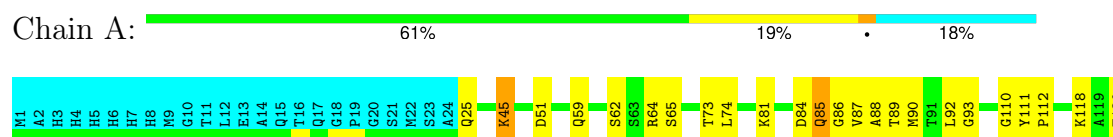
4.2.15 Score per residue for model 15

- Molecule 1: FKBP



4.2.16 Score per residue for model 16

- Molecule 1: FKBP

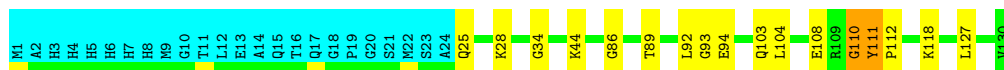




4.2.17 Score per residue for model 17

- Molecule 1: FKBP

Chain A: 68% 12% 18%



4.2.18 Score per residue for model 18

- Molecule 1: FKBP

Chain A: 68% 12% 18%



4.2.19 Score per residue for model 19

- Molecule 1: FKBP

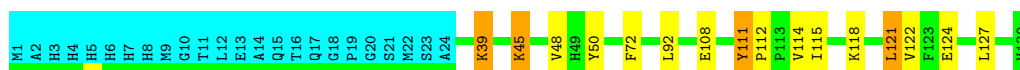
Chain A: 65% 15% 18%



4.2.20 Score per residue for model 20

- Molecule 1: FKBP

Chain A: 69% 9% 18%



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: *target function*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CYANA | structure solution | 3.0 |
| CNS | refinement | 1.1 |
| CYANA | 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 | 1218 |
| Number of shifts mapped to atoms | 1218 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 77% |

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 | 819 | 833 | 832 | 10±2 |
| All | All | 16380 | 16660 | 16640 | 199 |

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 6.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:90:MET:SD | 1:A:127:LEU:HB2 | 0.77 | 2.19 | 4 | 10 |
| 1:A:92:LEU:HA | 1:A:127:LEU:HD12 | 0.71 | 1.62 | 8 | 17 |
| 1:A:51:ASP:HB2 | 1:A:124:GLU:HB2 | 0.66 | 1.65 | 11 | 6 |
| 1:A:81:LYS:HA | 1:A:84:ASP:HB3 | 0.64 | 1.69 | 8 | 7 |
| 1:A:48:VAL:HG12 | 1:A:127:LEU:HD22 | 0.63 | 1.71 | 11 | 5 |
| 1:A:51:ASP:HB3 | 1:A:124:GLU:HB3 | 0.63 | 1.70 | 9 | 2 |
| 1:A:111:TYR:HB2 | 1:A:112:PRO:HD3 | 0.63 | 1.71 | 12 | 16 |
| 1:A:108:GLU:HA | 1:A:118:LYS:HA | 0.61 | 1.72 | 15 | 3 |
| 1:A:118:LYS:NZ | 1:A:118:LYS:HB2 | 0.60 | 2.11 | 3 | 2 |
| 1:A:28:LYS:N | 1:A:28:LYS:HD3 | 0.59 | 2.11 | 3 | 1 |
| 1:A:85:GLN:HE21 | 1:A:85:GLN:HA | 0.58 | 1.57 | 16 | 1 |
| 1:A:49:HIS:CE1 | 1:A:64:ARG:HA | 0.58 | 2.33 | 1 | 2 |
| 1:A:74:LEU:HD11 | 1:A:88:ALA:HB2 | 0.58 | 1.73 | 3 | 2 |
| 1:A:49:HIS:HB2 | 1:A:126:GLU:HB3 | 0.56 | 1.77 | 13 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:45:LYS:HB2 | 1:A:45:LYS:HZ3 | 0.53 | 1.63 | 20 | 2 |
| 1:A:49:HIS:HB3 | 1:A:126:GLU:HB3 | 0.53 | 1.81 | 1 | 3 |
| 1:A:87:VAL:O | 1:A:90:MET:HG2 | 0.53 | 2.04 | 6 | 8 |
| 1:A:112:PRO:HG2 | 1:A:115:ILE:HB | 0.53 | 1.81 | 13 | 1 |
| 1:A:121:LEU:HD13 | 1:A:122:VAL:N | 0.52 | 2.19 | 15 | 15 |
| 1:A:86:GLY:O | 1:A:89:THR:HG22 | 0.51 | 2.06 | 19 | 5 |
| 1:A:27:GLU:HB3 | 1:A:29:LYS:HE3 | 0.51 | 1.83 | 7 | 1 |
| 1:A:51:ASP:HA | 1:A:63:SER:HB2 | 0.51 | 1.81 | 8 | 3 |
| 1:A:25:GLN:HB2 | 1:A:120:THR:HG21 | 0.51 | 1.81 | 16 | 1 |
| 1:A:114:VAL:HG23 | 1:A:115:ILE:HG12 | 0.50 | 1.84 | 13 | 3 |
| 1:A:80:ILE:HD12 | 1:A:105:ALA:HA | 0.49 | 1.85 | 8 | 1 |
| 1:A:45:LYS:HD2 | 1:A:71:GLN:HB3 | 0.49 | 1.83 | 13 | 1 |
| 1:A:52:GLY:O | 1:A:59:GLN:HB2 | 0.49 | 2.08 | 19 | 2 |
| 1:A:110:GLY:O | 1:A:111:TYR:HB2 | 0.49 | 2.07 | 5 | 4 |
| 1:A:31:LEU:HD23 | 1:A:95:LYS:HD3 | 0.48 | 1.84 | 5 | 1 |
| 1:A:28:LYS:HB2 | 1:A:28:LYS:HZ2 | 0.48 | 1.66 | 11 | 1 |
| 1:A:50:TYR:HA | 1:A:124:GLU:O | 0.48 | 2.09 | 20 | 3 |
| 1:A:31:LEU:HD11 | 1:A:97:LEU:HB2 | 0.47 | 1.87 | 19 | 1 |
| 1:A:66:ARG:HA | 1:A:66:ARG:HE | 0.47 | 1.69 | 3 | 1 |
| 1:A:45:LYS:NZ | 1:A:73:THR:OG1 | 0.47 | 2.48 | 16 | 1 |
| 1:A:53:ARG:HG3 | 1:A:59:GLN:HB3 | 0.46 | 1.86 | 9 | 2 |
| 1:A:101:PRO:HA | 1:A:120:THR:HG23 | 0.46 | 1.87 | 11 | 3 |
| 1:A:111:TYR:H | 1:A:112:PRO:HD2 | 0.46 | 1.71 | 18 | 1 |
| 1:A:28:LYS:HD3 | 1:A:28:LYS:H | 0.46 | 1.71 | 4 | 1 |
| 1:A:116:PRO:HG2 | 1:A:119:ALA:HB2 | 0.46 | 1.86 | 12 | 1 |
| 1:A:34:GLY:HA3 | 1:A:94:GLU:HB2 | 0.46 | 1.87 | 12 | 5 |
| 1:A:49:HIS:ND1 | 1:A:128:LEU:HD21 | 0.45 | 2.25 | 13 | 1 |
| 1:A:110:GLY:O | 1:A:112:PRO:HD2 | 0.45 | 2.11 | 5 | 2 |
| 1:A:39:LYS:HB3 | 1:A:39:LYS:NZ | 0.45 | 2.26 | 6 | 2 |
| 1:A:62:SER:OG | 1:A:64:ARG:HG3 | 0.45 | 2.10 | 16 | 1 |
| 1:A:92:LEU:HD23 | 1:A:93:GLY:N | 0.44 | 2.25 | 16 | 4 |
| 1:A:64:ARG:HD2 | 1:A:65:SER:N | 0.44 | 2.28 | 16 | 1 |
| 1:A:118:LYS:HB3 | 1:A:118:LYS:NZ | 0.44 | 2.28 | 16 | 1 |
| 1:A:28:LYS:HB3 | 1:A:98:PHE:CD2 | 0.44 | 2.48 | 9 | 1 |
| 1:A:25:GLN:H | 1:A:101:PRO:HB3 | 0.43 | 1.72 | 2 | 1 |
| 1:A:38:THR:O | 1:A:40:PRO:HD3 | 0.43 | 2.13 | 7 | 1 |
| 1:A:127:LEU:HD11 | 1:A:130:VAL:HB | 0.43 | 1.90 | 14 | 1 |
| 1:A:53:ARG:NH2 | 1:A:64:ARG:NH2 | 0.43 | 2.66 | 8 | 1 |
| 1:A:112:PRO:HD2 | 1:A:115:ILE:HB | 0.43 | 1.91 | 12 | 1 |
| 1:A:49:HIS:HB2 | 1:A:128:LEU:HD21 | 0.43 | 1.91 | 1 | 1 |
| 1:A:87:VAL:HG23 | 1:A:127:LEU:HD23 | 0.43 | 1.89 | 11 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:79:VAL:HB | 1:A:83:TRP:HE3 | 0.43 | 1.73 | 1 | 1 |
| 1:A:35:ASP:HB3 | 1:A:37:VAL:HG22 | 0.43 | 1.91 | 8 | 1 |
| 1:A:59:GLN:NE2 | 1:A:62:SER:HA | 0.43 | 2.29 | 19 | 1 |
| 1:A:49:HIS:HB3 | 1:A:128:LEU:HD21 | 0.43 | 1.90 | 3 | 1 |
| 1:A:38:THR:HG21 | 1:A:92:LEU:HB2 | 0.42 | 1.90 | 18 | 1 |
| 1:A:103:GLN:HG3 | 1:A:104:LEU:HG | 0.42 | 1.90 | 17 | 1 |
| 1:A:100:ILE:HG22 | 1:A:105:ALA:HB2 | 0.42 | 1.92 | 8 | 1 |
| 1:A:30:VAL:HA | 1:A:96:ALA:HA | 0.42 | 1.91 | 1 | 1 |
| 1:A:81:LYS:HD3 | 1:A:81:LYS:O | 0.42 | 2.15 | 1 | 2 |
| 1:A:28:LYS:NZ | 1:A:89:THR:OG1 | 0.42 | 2.51 | 14 | 1 |
| 1:A:64:ARG:HG2 | 1:A:65:SER:N | 0.42 | 2.30 | 14 | 1 |
| 1:A:118:LYS:HB2 | 1:A:118:LYS:HZ2 | 0.42 | 1.73 | 3 | 1 |
| 1:A:68:LYS:HD2 | 1:A:69:PRO:HD2 | 0.42 | 1.92 | 5 | 1 |
| 1:A:51:ASP:O | 1:A:123:PHE:HA | 0.42 | 2.14 | 13 | 1 |
| 1:A:58:LYS:NZ | 1:A:58:LYS:HB2 | 0.41 | 2.30 | 2 | 1 |
| 1:A:80:ILE:HD12 | 1:A:104:LEU:O | 0.41 | 2.14 | 14 | 1 |
| 1:A:39:LYS:NZ | 1:A:39:LYS:HB2 | 0.41 | 2.30 | 2 | 2 |
| 1:A:108:GLU:HG3 | 1:A:109:ARG:N | 0.41 | 2.30 | 7 | 1 |
| 1:A:51:ASP:HB3 | 1:A:124:GLU:HB2 | 0.41 | 1.92 | 7 | 1 |
| 1:A:48:VAL:HG11 | 1:A:87:VAL:HG21 | 0.41 | 1.92 | 5 | 1 |
| 1:A:111:TYR:CB | 1:A:112:PRO:HD3 | 0.41 | 2.44 | 15 | 1 |
| 1:A:45:LYS:HA | 1:A:73:THR:HA | 0.41 | 1.93 | 16 | 1 |
| 1:A:41:GLN:HG2 | 1:A:44:LYS:HE2 | 0.41 | 1.93 | 18 | 1 |
| 1:A:92:LEU:HD12 | 1:A:130:VAL:HG23 | 0.41 | 1.92 | 2 | 1 |
| 1:A:29:LYS:HB2 | 1:A:97:LEU:HB3 | 0.41 | 1.92 | 5 | 1 |
| 1:A:50:TYR:HD1 | 1:A:125:VAL:HG12 | 0.41 | 1.75 | 12 | 1 |
| 1:A:92:LEU:HD23 | 1:A:130:VAL:HG12 | 0.41 | 1.93 | 14 | 1 |
| 1:A:48:VAL:HG21 | 1:A:72:PHE:CE2 | 0.41 | 2.50 | 20 | 1 |
| 1:A:28:LYS:HD3 | 1:A:28:LYS:N | 0.40 | 2.31 | 2 | 1 |
| 1:A:45:LYS:HB2 | 1:A:45:LYS:NZ | 0.40 | 2.30 | 10 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|-----|-------|-----------------|---------------|------------|------------|-------------|
| 1 | A | 105/130 (81%) | 101±2 (96±2%) | 3±2 (3±2%) | 1±0 (1±0%) | 17 67 |
| All | All | 2100/2600 (81%) | 2024 (96%) | 57 (3%) | 19 (1%) | 17 67 |

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

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 111 | TYR | 17 |
| 1 | A | 110 | GLY | 2 |

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 | 86/104 (83%) | 83±1 (97±1%) | 3±1 (3±1%) | 34 85 |
| All | All | 1720/2080 (83%) | 1662 (97%) | 58 (3%) | 34 85 |

All 20 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 | 121 | LEU | 15 |
| 1 | A | 28 | LYS | 7 |
| 1 | A | 127 | LEU | 6 |
| 1 | A | 64 | ARG | 6 |
| 1 | A | 45 | LYS | 3 |
| 1 | A | 109 | ARG | 2 |
| 1 | A | 51 | ASP | 2 |
| 1 | A | 39 | LYS | 2 |
| 1 | A | 92 | LEU | 2 |
| 1 | A | 31 | LEU | 2 |
| 1 | A | 44 | LYS | 2 |
| 1 | A | 35 | ASP | 1 |
| 1 | A | 61 | ASP | 1 |
| 1 | A | 68 | LYS | 1 |
| 1 | A | 53 | ARG | 1 |
| 1 | A | 84 | ASP | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 59 | GLN | 1 |
| 1 | A | 85 | GLN | 1 |
| 1 | A | 29 | LYS | 1 |
| 1 | A | 25 | GLN | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 70% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

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

| | |
|---|------|
| Total number of shifts | 1218 |
| Number of shifts mapped to atoms | 1218 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 1 |

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 121 | -0.12 ± 0.18 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 104 | -0.12 ± 0.19 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 111 | -0.21 ± 0.51 | 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 77%, i.e. 1105 atoms were assigned a chemical shift out of a possible 1433. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone | 396/525 (75%) | 196/216 (91%) | 104/212 (49%) | 96/97 (99%) |
| Sidechain | 639/792 (81%) | 430/516 (83%) | 205/248 (83%) | 4/28 (14%) |

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| | Total | ¹H | ¹³C | ¹⁵N |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 70/116 (60%) | 38/56 (68%) | 31/57 (54%) | 1/3 (33%) |
| Overall | 1105/1433 (77%) | 664/788 (84%) | 340/517 (66%) | 101/128 (79%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 70%, i.e. 1217 atoms were assigned a chemical shift out of a possible 1729. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹H | ¹³C | ¹⁵N |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone | 457/646 (71%) | 225/266 (85%) | 121/260 (47%) | 111/120 (92%) |
| Sidechain | 690/919 (75%) | 460/601 (77%) | 226/288 (78%) | 4/30 (13%) |
| Aromatic | 70/164 (43%) | 38/80 (48%) | 31/69 (45%) | 1/15 (7%) |
| Overall | 1217/1729 (70%) | 723/947 (76%) | 378/617 (61%) | 116/165 (70%) |

7.1.4 Statistically unusual chemical shifts [i](#)

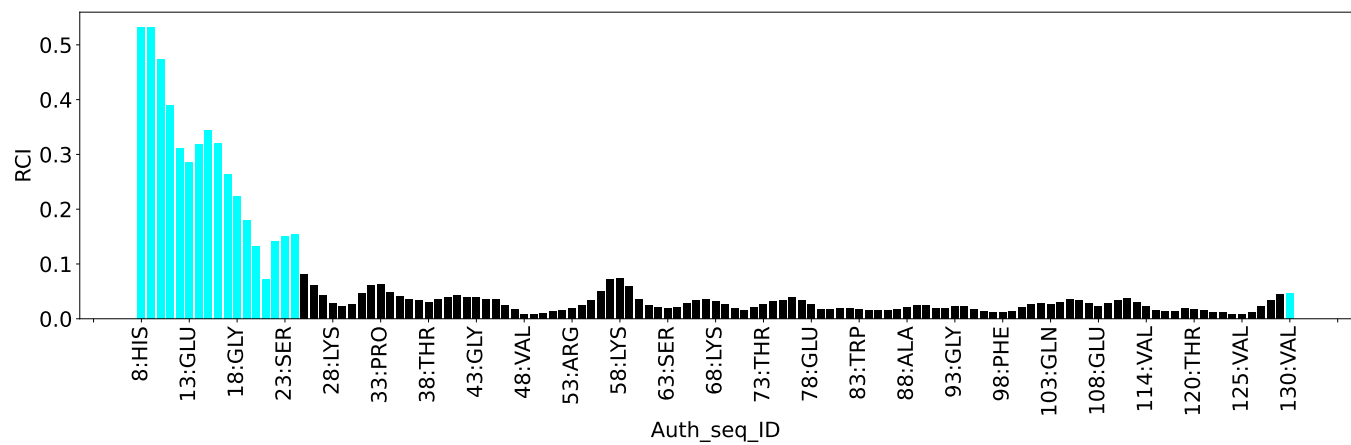
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 118 | LYS | HG3 | -0.09 | 0.04 – 2.67 | -5.5 |

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 | 1739 |
| Intra-residue ($ i-j =0$) | 395 |
| Sequential ($ i-j =1$) | 468 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 251 |
| Long range ($ i-j \geq 5$) | 549 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 76 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 150 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 14.5 |
| Number of long range restraints per residue ¹ | 4.7 |

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) | 44.5 | 0.2 |
| 0.2-0.5 (Medium) | 86.6 | 0.5 |
| >0.5 (Large) | 157.0 | 5.69 |

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

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

| Bins (°) | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small) | 0.1 | 1.85 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

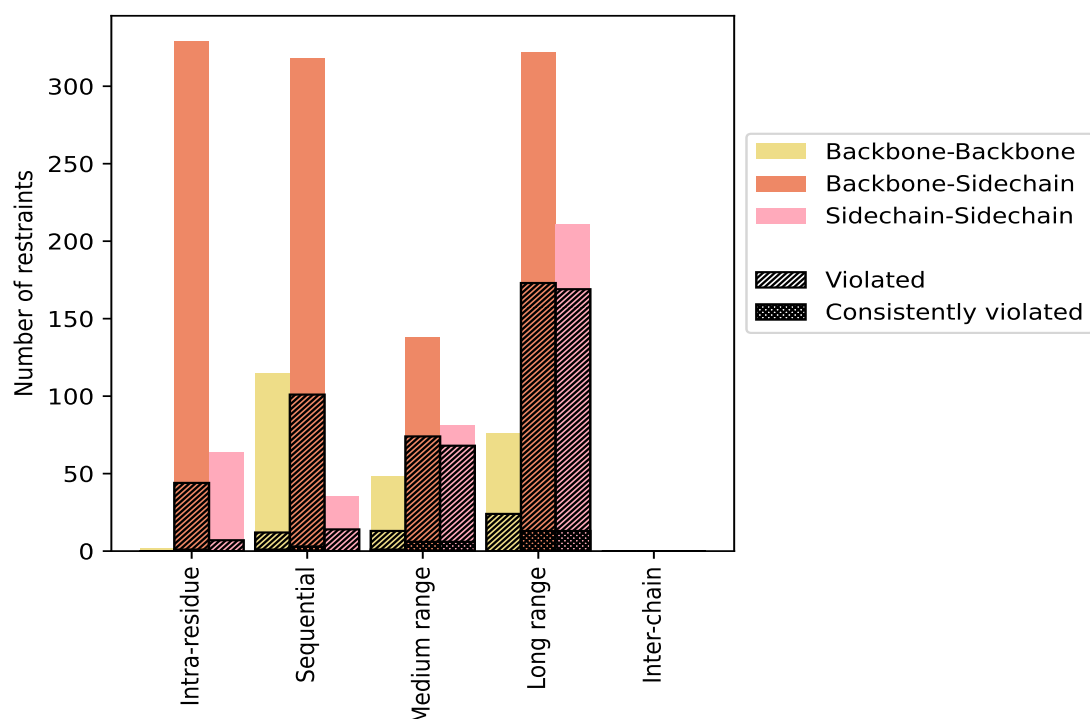
9.1 Summary of distance violations ⓘ

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 ($i-j =0$) | 395 | 22.7 | 51 | 12.9 | 2.9 | 1 | 0.3 | 0.1 |
| Backbone-Backbone | 2 | 0.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 329 | 18.9 | 44 | 13.4 | 2.5 | 1 | 0.3 | 0.1 |
| Sidechain-Sidechain | 64 | 3.7 | 7 | 10.9 | 0.4 | 0 | 0.0 | 0.0 |
| Sequential ($i-j =1$) | 468 | 26.9 | 127 | 27.1 | 7.3 | 4 | 0.9 | 0.2 |
| Backbone-Backbone | 115 | 6.6 | 12 | 10.4 | 0.7 | 1 | 0.9 | 0.1 |
| Backbone-Sidechain | 318 | 18.3 | 101 | 31.8 | 5.8 | 3 | 0.9 | 0.2 |
| Sidechain-Sidechain | 35 | 2.0 | 14 | 40.0 | 0.8 | 0 | 0.0 | 0.0 |
| Medium range ($i-j >1$ & $i-j <5$) | 251 | 14.4 | 155 | 61.8 | 8.9 | 13 | 5.2 | 0.7 |
| Backbone-Backbone | 48 | 2.8 | 13 | 27.1 | 0.7 | 1 | 2.1 | 0.1 |
| Backbone-Sidechain | 122 | 7.0 | 74 | 60.7 | 4.3 | 6 | 4.9 | 0.3 |
| Sidechain-Sidechain | 81 | 4.7 | 68 | 84.0 | 3.9 | 6 | 7.4 | 0.3 |
| Long range ($i-j \geq 5$) | 549 | 31.6 | 366 | 66.7 | 21.0 | 26 | 4.7 | 1.5 |
| Backbone-Backbone | 76 | 4.4 | 24 | 31.6 | 1.4 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 262 | 15.1 | 173 | 66.0 | 9.9 | 13 | 5.0 | 0.7 |
| Sidechain-Sidechain | 211 | 12.1 | 169 | 80.1 | 9.7 | 13 | 6.2 | 0.7 |
| 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 | 76 | 4.4 | 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 | 1739 | 100.0 | 699 | 40.2 | 40.2 | 44 | 2.5 | 2.5 |
| Backbone-Backbone | 241 | 13.9 | 49 | 20.3 | 2.8 | 2 | 0.8 | 0.1 |
| Backbone-Sidechain | 1107 | 63.7 | 392 | 35.4 | 22.5 | 23 | 2.1 | 1.3 |
| Sidechain-Sidechain | 391 | 22.5 | 258 | 66.0 | 14.8 | 19 | 4.9 | 1.1 |

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 | 12 | 49 | 54 | 181 | 0 | 296 | 0.88 | 3.51 | 0.74 | 0.64 |
| 2 | 15 | 38 | 73 | 160 | 0 | 286 | 0.85 | 4.95 | 0.84 | 0.56 |
| 3 | 13 | 51 | 72 | 177 | 0 | 313 | 0.98 | 4.66 | 0.91 | 0.68 |
| 4 | 16 | 50 | 70 | 196 | 0 | 332 | 0.96 | 4.98 | 0.89 | 0.64 |
| 5 | 16 | 40 | 52 | 143 | 0 | 251 | 0.89 | 5.15 | 0.91 | 0.57 |
| 6 | 10 | 52 | 64 | 166 | 0 | 292 | 0.75 | 4.56 | 0.77 | 0.5 |
| 7 | 17 | 47 | 56 | 176 | 0 | 296 | 0.98 | 5.38 | 0.91 | 0.66 |
| 8 | 14 | 42 | 73 | 152 | 0 | 281 | 0.87 | 5.4 | 0.91 | 0.58 |
| 9 | 12 | 50 | 74 | 169 | 0 | 305 | 0.95 | 5.47 | 0.93 | 0.55 |
| 10 | 11 | 41 | 61 | 157 | 0 | 270 | 0.87 | 4.2 | 0.86 | 0.5 |

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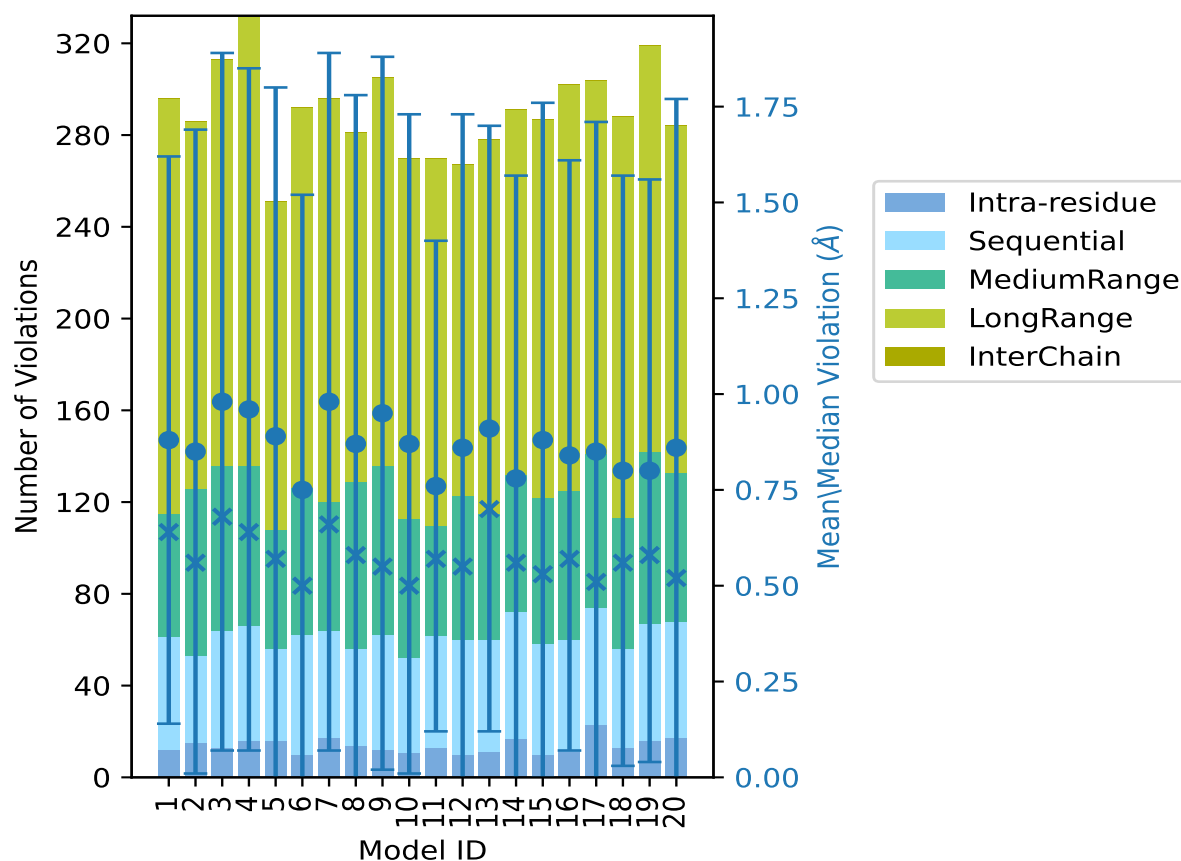
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 13 | 49 | 48 | 160 | 0 | 270 | 0.76 | 3.16 | 0.64 | 0.57 |
| 12 | 10 | 50 | 63 | 144 | 0 | 267 | 0.86 | 4.97 | 0.87 | 0.55 |
| 13 | 11 | 49 | 55 | 163 | 0 | 278 | 0.91 | 4.91 | 0.79 | 0.7 |
| 14 | 17 | 55 | 60 | 159 | 0 | 291 | 0.78 | 5.18 | 0.79 | 0.56 |
| 15 | 10 | 48 | 64 | 165 | 0 | 287 | 0.88 | 4.3 | 0.88 | 0.53 |
| 16 | 11 | 49 | 65 | 177 | 0 | 302 | 0.84 | 4.24 | 0.77 | 0.57 |
| 17 | 23 | 51 | 67 | 163 | 0 | 304 | 0.85 | 4.6 | 0.86 | 0.51 |
| 18 | 13 | 43 | 57 | 175 | 0 | 288 | 0.8 | 4.49 | 0.77 | 0.56 |
| 19 | 16 | 51 | 75 | 177 | 0 | 319 | 0.8 | 4.47 | 0.76 | 0.58 |
| 20 | 17 | 51 | 65 | 151 | 0 | 284 | 0.86 | 5.69 | 0.91 | 0.52 |

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

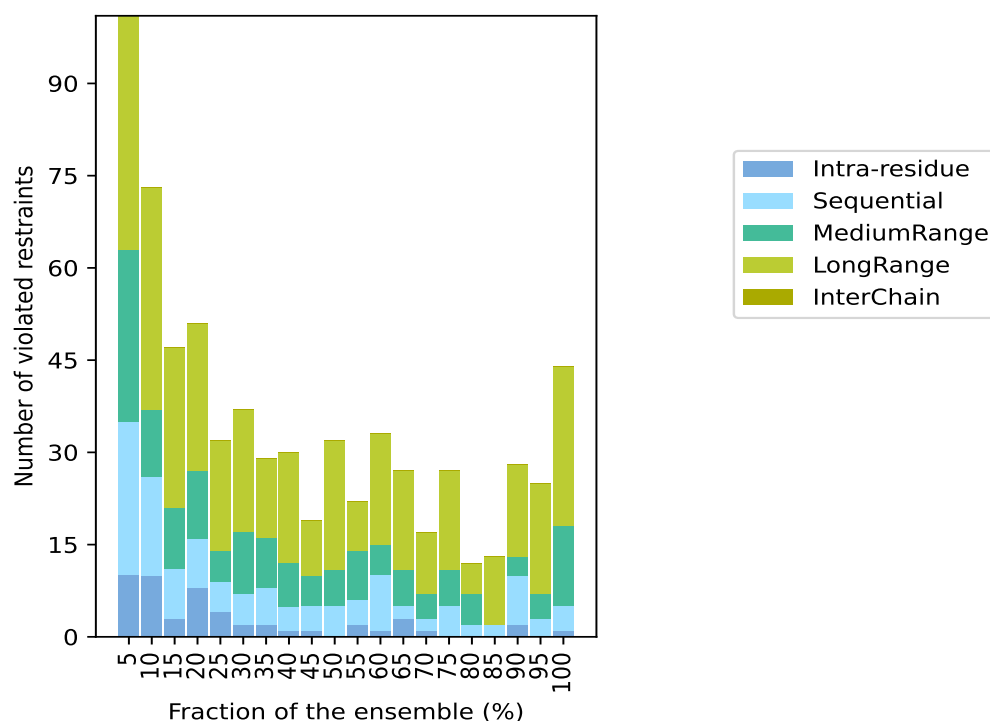
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 964(IR:344, SQ:341, MR:96, LR:183, IC:0) restraints are not 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 | % |
| 10 | 25 | 28 | 38 | 0 | 101 | 1 | 5.0 |
| 10 | 16 | 11 | 36 | 0 | 73 | 2 | 10.0 |
| 3 | 8 | 10 | 26 | 0 | 47 | 3 | 15.0 |
| 8 | 8 | 11 | 24 | 0 | 51 | 4 | 20.0 |
| 4 | 5 | 5 | 18 | 0 | 32 | 5 | 25.0 |
| 2 | 5 | 10 | 20 | 0 | 37 | 6 | 30.0 |
| 2 | 6 | 8 | 13 | 0 | 29 | 7 | 35.0 |
| 1 | 4 | 7 | 18 | 0 | 30 | 8 | 40.0 |
| 1 | 4 | 5 | 9 | 0 | 19 | 9 | 45.0 |
| 0 | 5 | 6 | 21 | 0 | 32 | 10 | 50.0 |
| 2 | 4 | 8 | 8 | 0 | 22 | 11 | 55.0 |
| 1 | 9 | 5 | 18 | 0 | 33 | 12 | 60.0 |
| 3 | 2 | 6 | 16 | 0 | 27 | 13 | 65.0 |
| 1 | 2 | 4 | 10 | 0 | 17 | 14 | 70.0 |
| 0 | 5 | 6 | 16 | 0 | 27 | 15 | 75.0 |
| 0 | 2 | 5 | 5 | 0 | 12 | 16 | 80.0 |
| 0 | 2 | 0 | 11 | 0 | 13 | 17 | 85.0 |
| 2 | 8 | 3 | 15 | 0 | 28 | 18 | 90.0 |
| 0 | 3 | 4 | 18 | 0 | 25 | 19 | 95.0 |
| 1 | 4 | 13 | 26 | 0 | 44 | 20 | 100.0 |

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

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

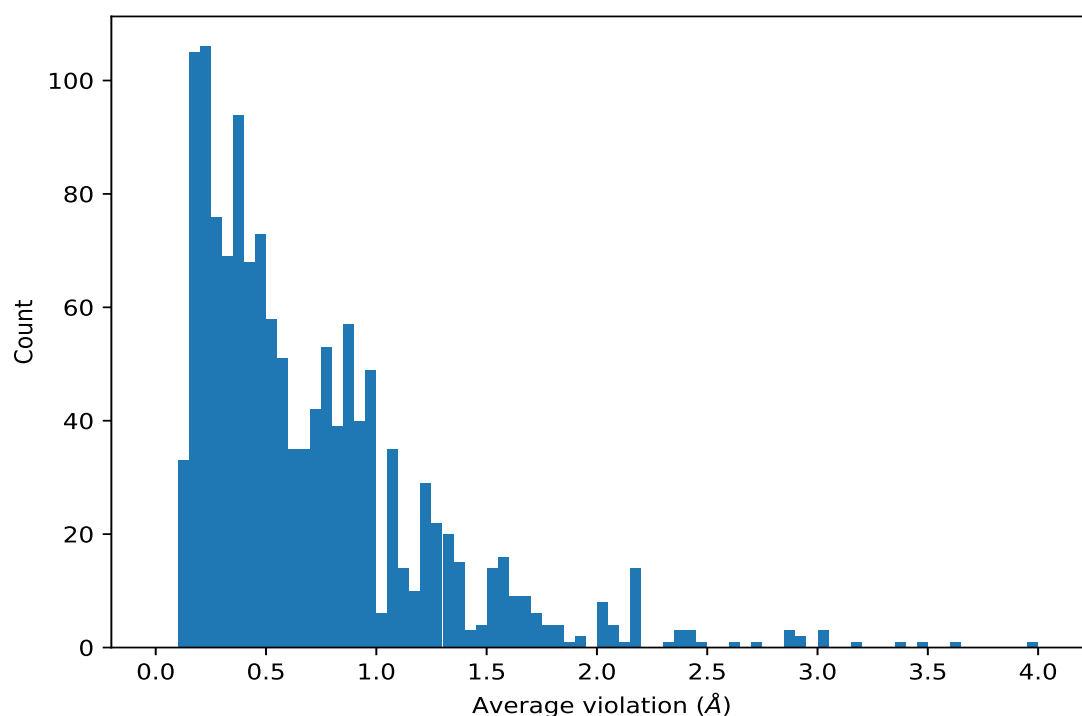
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 20 | 3.96 | 0.9 | 4.05 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 20 | 3.62 | 0.9 | 3.67 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 20 | 3.49 | 1.31 | 3.89 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 20 | 3.38 | 0.83 | 3.44 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 20 | 2.9 | 1.11 | 3.11 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 20 | 2.9 | 1.11 | 3.11 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 20 | 1.91 | 0.65 | 1.62 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 20 | 1.89 | 0.87 | 1.93 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 20 | 1.74 | 0.43 | 1.88 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 20 | 1.72 | 0.74 | 1.9 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 20 | 1.69 | 0.56 | 1.81 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 20 | 1.66 | 1.0 | 1.52 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 20 | 1.59 | 0.43 | 1.86 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 20 | 1.51 | 0.37 | 1.54 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 20 | 1.51 | 0.37 | 1.54 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 20 | 1.51 | 0.37 | 1.54 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 20 | 1.51 | 0.56 | 1.66 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 20 | 1.51 | 0.56 | 1.66 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 20 | 1.51 | 0.56 | 1.66 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 20 | 1.51 | 0.56 | 1.66 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 20 | 1.51 | 0.56 | 1.66 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 20 | 1.51 | 0.56 | 1.66 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 20 | 1.48 | 0.59 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 20 | 1.48 | 0.59 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 20 | 1.48 | 0.59 | 1.28 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 20 | 1.38 | 0.68 | 1.1 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 20 | 1.36 | 0.46 | 1.27 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 20 | 1.36 | 0.46 | 1.27 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 20 | 1.36 | 0.46 | 1.27 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 20 | 1.34 | 0.74 | 1.2 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 20 | 1.34 | 0.74 | 1.2 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 20 | 1.34 | 0.74 | 1.2 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 20 | 1.33 | 0.55 | 1.3 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 20 | 1.16 | 0.31 | 1.14 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 20 | 1.16 | 0.31 | 1.14 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 20 | 1.16 | 0.31 | 1.14 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 20 | 1.12 | 0.26 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 20 | 1.12 | 0.26 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 20 | 1.12 | 0.26 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 20 | 1.12 | 0.26 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 20 | 1.12 | 0.26 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 20 | 1.12 | 0.26 | 1.13 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 20 | 1.09 | 0.36 | 1.04 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 20 | 1.09 | 0.36 | 1.04 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 20 | 1.09 | 0.36 | 1.04 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 20 | 1.08 | 0.48 | 0.98 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 20 | 1.08 | 0.45 | 1.05 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 20 | 1.08 | 0.45 | 1.05 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 20 | 1.08 | 0.45 | 1.05 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 20 | 1.08 | 0.45 | 1.05 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 20 | 1.08 | 0.45 | 1.05 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 20 | 1.08 | 0.45 | 1.05 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 20 | 1.06 | 0.69 | 0.94 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 20 | 1.06 | 0.69 | 0.94 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 20 | 1.06 | 0.69 | 0.94 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 20 | 0.98 | 0.37 | 0.95 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 20 | 0.97 | 0.28 | 1.0 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 20 | 0.94 | 0.6 | 0.8 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 20 | 0.94 | 0.6 | 0.8 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 20 | 0.94 | 0.6 | 0.8 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 20 | 0.92 | 0.39 | 0.8 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 20 | 0.92 | 0.39 | 0.8 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 20 | 0.92 | 0.39 | 0.8 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 20 | 0.9 | 0.61 | 0.6 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 20 | 0.87 | 0.46 | 1.02 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 20 | 0.87 | 0.46 | 1.02 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 20 | 0.87 | 0.46 | 1.02 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 20 | 0.86 | 0.5 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 20 | 0.86 | 0.5 | 0.81 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 20 | 0.85 | 0.32 | 0.79 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 20 | 0.78 | 0.38 | 0.64 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 20 | 0.75 | 0.39 | 0.72 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 20 | 0.75 | 0.39 | 0.72 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 20 | 0.75 | 0.39 | 0.72 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 20 | 0.72 | 0.33 | 0.79 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 20 | 0.69 | 0.25 | 0.62 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 20 | 0.65 | 0.17 | 0.63 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 20 | 0.65 | 0.17 | 0.63 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 20 | 0.65 | 0.17 | 0.63 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 20 | 0.61 | 0.38 | 0.51 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 20 | 0.61 | 0.38 | 0.51 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 20 | 0.61 | 0.38 | 0.51 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 20 | 0.43 | 0.1 | 0.46 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 20 | 0.39 | 0.18 | 0.34 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 20 | 0.39 | 0.18 | 0.34 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 20 | 0.35 | 0.02 | 0.36 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 20 | 0.25 | 0.05 | 0.26 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 20 | 0.25 | 0.05 | 0.26 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 20 | 0.25 | 0.05 | 0.26 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 20 | 0.22 | 0.05 | 0.23 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 19 | 2.85 | 0.69 | 2.8 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 19 | 2.85 | 0.69 | 2.8 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 19 | 2.85 | 0.69 | 2.8 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 19 | 2.39 | 0.68 | 2.21 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 19 | 2.19 | 1.12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 19 | 2.19 | 1.12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 19 | 2.19 | 1.12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 19 | 2.19 | 1.12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 19 | 2.19 | 1.12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 19 | 2.19 | 1.12 | 1.9 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 19 | 1.77 | 1.0 | 1.76 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 19 | 1.63 | 0.76 | 1.51 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 19 | 1.63 | 0.76 | 1.51 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 19 | 1.63 | 0.76 | 1.51 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 19 | 1.55 | 0.82 | 1.54 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 19 | 1.55 | 0.66 | 1.77 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 19 | 1.55 | 0.66 | 1.77 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 19 | 1.55 | 0.66 | 1.77 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 19 | 1.33 | 0.59 | 1.27 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 19 | 1.25 | 0.45 | 1.24 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 19 | 1.25 | 0.45 | 1.24 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 19 | 1.25 | 0.45 | 1.24 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 19 | 1.23 | 0.69 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 19 | 1.23 | 0.69 | 1.14 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 19 | 1.21 | 1.16 | 1.04 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 19 | 1.17 | 0.57 | 1.08 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 19 | 0.99 | 0.35 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 19 | 0.99 | 0.35 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 19 | 0.99 | 0.35 | 1.02 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 19 | 0.99 | 0.35 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 19 | 0.99 | 0.35 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 19 | 0.99 | 0.35 | 1.02 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 19 | 0.93 | 0.58 | 0.81 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 19 | 0.82 | 0.24 | 0.88 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 19 | 0.82 | 0.24 | 0.88 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 19 | 0.82 | 0.24 | 0.88 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 19 | 0.79 | 0.42 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 19 | 0.79 | 0.42 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 19 | 0.79 | 0.42 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 19 | 0.79 | 0.42 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 19 | 0.79 | 0.42 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 19 | 0.79 | 0.42 | 0.73 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 19 | 0.79 | 0.29 | 0.75 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 19 | 0.79 | 0.29 | 0.75 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 19 | 0.79 | 0.29 | 0.75 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 19 | 0.78 | 0.21 | 0.86 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 19 | 0.76 | 0.3 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 19 | 0.76 | 0.3 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 19 | 0.76 | 0.3 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 19 | 0.76 | 0.3 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 19 | 0.76 | 0.3 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 19 | 0.76 | 0.3 | 0.75 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 19 | 0.75 | 0.25 | 0.72 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 19 | 0.65 | 0.38 | 0.53 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 19 | 0.58 | 0.25 | 0.64 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 19 | 0.42 | 0.26 | 0.38 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 19 | 0.29 | 0.09 | 0.27 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 19 | 0.21 | 0.04 | 0.22 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 18 | 3.18 | 0.75 | 3.3 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 18 | 2.44 | 0.66 | 2.28 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 18 | 2.31 | 0.92 | 2.7 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 18 | 2.19 | 0.83 | 1.99 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 18 | 2.19 | 0.83 | 1.99 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 18 | 2.19 | 0.83 | 1.99 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 18 | 2.18 | 1.22 | 2.2 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 18 | 2.18 | 1.22 | 2.2 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 18 | 2.18 | 1.22 | 2.2 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 18 | 2.12 | 0.49 | 1.98 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 18 | 2.01 | 0.31 | 1.92 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 18 | 2.01 | 0.31 | 1.92 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 18 | 1.5 | 0.73 | 1.59 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 18 | 1.35 | 0.2 | 1.32 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 18 | 1.35 | 0.2 | 1.32 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 18 | 1.35 | 0.2 | 1.32 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 18 | 1.31 | 0.5 | 1.28 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 18 | 1.09 | 0.74 | 1.0 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 18 | 1.09 | 0.74 | 1.0 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 18 | 1.09 | 0.74 | 1.0 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 18 | 1.09 | 0.74 | 1.0 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 18 | 1.09 | 0.74 | 1.0 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 18 | 1.09 | 0.74 | 1.0 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 18 | 0.96 | 0.53 | 0.93 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 18 | 0.88 | 0.43 | 0.84 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 18 | 0.88 | 0.43 | 0.84 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 18 | 0.88 | 0.43 | 0.84 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 18 | 0.8 | 0.47 | 0.67 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 18 | 0.8 | 0.47 | 0.67 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 18 | 0.8 | 0.47 | 0.67 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 18 | 0.72 | 0.38 | 0.7 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 18 | 0.62 | 0.36 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 18 | 0.62 | 0.36 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 18 | 0.62 | 0.36 | 0.56 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 18 | 0.59 | 0.21 | 0.5 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 18 | 0.58 | 0.26 | 0.62 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 18 | 0.58 | 0.26 | 0.62 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 18 | 0.58 | 0.26 | 0.62 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 18 | 0.53 | 0.21 | 0.5 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 18 | 0.53 | 0.21 | 0.5 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 18 | 0.53 | 0.21 | 0.5 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 18 | 0.49 | 0.21 | 0.5 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 18 | 0.47 | 0.19 | 0.48 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 18 | 0.44 | 0.21 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 18 | 0.44 | 0.21 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 18 | 0.44 | 0.21 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 18 | 0.44 | 0.21 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 18 | 0.44 | 0.21 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 18 | 0.44 | 0.21 | 0.38 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 18 | 0.35 | 0.15 | 0.32 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 18 | 0.33 | 0.13 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 18 | 0.33 | 0.13 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 18 | 0.33 | 0.13 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 18 | 0.33 | 0.13 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 18 | 0.33 | 0.13 | 0.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 18 | 0.33 | 0.13 | 0.36 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 18 | 0.29 | 0.12 | 0.34 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 18 | 0.25 | 0.1 | 0.22 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 18 | 0.25 | 0.1 | 0.22 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 18 | 0.21 | 0.07 | 0.22 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 18 | 0.21 | 0.07 | 0.22 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 18 | 0.21 | 0.07 | 0.22 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 18 | 0.17 | 0.02 | 0.18 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 17 | 1.62 | 0.88 | 1.65 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 17 | 1.62 | 0.88 | 1.65 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 17 | 1.62 | 0.88 | 1.65 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 17 | 1.57 | 0.82 | 1.29 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 17 | 1.57 | 0.82 | 1.29 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 17 | 1.57 | 0.82 | 1.29 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 17 | 1.31 | 0.53 | 1.41 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 17 | 1.31 | 0.53 | 1.41 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 17 | 1.31 | 0.53 | 1.41 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 17 | 1.11 | 0.57 | 1.13 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 17 | 1.11 | 0.57 | 1.13 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 17 | 1.11 | 0.57 | 1.13 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 17 | 1.04 | 0.7 | 0.84 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 17 | 0.96 | 0.75 | 0.6 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 17 | 0.96 | 0.75 | 0.6 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 17 | 0.66 | 0.39 | 0.56 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 17 | 0.66 | 0.39 | 0.56 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 17 | 0.66 | 0.39 | 0.56 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 17 | 0.63 | 0.29 | 0.61 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 17 | 0.56 | 0.31 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 17 | 0.56 | 0.31 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 17 | 0.56 | 0.31 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 17 | 0.56 | 0.31 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 17 | 0.56 | 0.31 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 17 | 0.56 | 0.31 | 0.6 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 17 | 0.48 | 0.3 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 17 | 0.48 | 0.3 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 17 | 0.48 | 0.3 | 0.46 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 17 | 0.46 | 0.13 | 0.49 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 17 | 0.46 | 0.13 | 0.49 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 17 | 0.36 | 0.11 | 0.39 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 17 | 0.36 | 0.11 | 0.39 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 17 | 0.36 | 0.11 | 0.39 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 17 | 0.23 | 0.1 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 17 | 0.23 | 0.1 | 0.2 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 17 | 0.23 | 0.1 | 0.2 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 16 | 1.61 | 0.96 | 1.59 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 16 | 1.61 | 0.96 | 1.59 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 16 | 1.61 | 0.96 | 1.59 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 16 | 1.56 | 0.93 | 1.62 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 16 | 1.56 | 0.84 | 1.81 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 16 | 1.44 | 0.71 | 1.41 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 16 | 1.4 | 0.68 | 1.38 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 16 | 0.85 | 0.4 | 1.04 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 16 | 0.82 | 0.46 | 0.76 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 16 | 0.76 | 0.65 | 0.7 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 16 | 0.76 | 0.65 | 0.7 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 16 | 0.76 | 0.65 | 0.7 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 16 | 0.64 | 0.36 | 0.61 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 16 | 0.52 | 0.22 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 16 | 0.52 | 0.22 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 16 | 0.52 | 0.22 | 0.54 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 16 | 0.4 | 0.19 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 16 | 0.4 | 0.19 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 16 | 0.4 | 0.19 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 16 | 0.4 | 0.19 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 16 | 0.4 | 0.19 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 16 | 0.4 | 0.19 | 0.4 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 16 | 0.32 | 0.08 | 0.32 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 15 | 2.49 | 1.31 | 2.33 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 15 | 2.17 | 0.95 | 2.3 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 15 | 2.17 | 0.95 | 2.3 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 15 | 1.94 | 1.64 | 0.98 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 15 | 1.22 | 0.32 | 1.26 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 15 | 1.08 | 0.51 | 1.14 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 15 | 0.96 | 0.44 | 0.9 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 15 | 0.96 | 0.57 | 0.83 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 15 | 0.96 | 0.57 | 0.83 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 15 | 0.96 | 0.57 | 0.83 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 15 | 0.95 | 0.46 | 0.94 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 15 | 0.95 | 0.46 | 0.94 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 15 | 0.92 | 0.38 | 0.9 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 15 | 0.92 | 0.38 | 0.9 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 15 | 0.92 | 0.38 | 0.9 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 15 | 0.9 | 0.64 | 0.5 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 15 | 0.89 | 0.52 | 0.73 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 15 | 0.89 | 0.52 | 0.73 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 15 | 0.85 | 0.21 | 0.89 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 15 | 0.85 | 0.21 | 0.89 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 15 | 0.85 | 0.21 | 0.89 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 15 | 0.81 | 0.81 | 0.54 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 15 | 0.81 | 0.81 | 0.54 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 15 | 0.81 | 0.81 | 0.54 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 15 | 0.81 | 0.56 | 0.49 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 15 | 0.79 | 0.32 | 0.68 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 15 | 0.78 | 0.4 | 0.68 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 15 | 0.78 | 0.4 | 0.68 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 15 | 0.78 | 0.4 | 0.68 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 15 | 0.76 | 0.52 | 0.72 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 15 | 0.76 | 0.52 | 0.72 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 15 | 0.76 | 0.52 | 0.72 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 15 | 0.74 | 0.62 | 0.48 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 15 | 0.74 | 0.62 | 0.48 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 15 | 0.74 | 0.62 | 0.48 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 15 | 0.72 | 0.44 | 0.67 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 15 | 0.66 | 0.55 | 0.37 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 15 | 0.66 | 0.55 | 0.37 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 15 | 0.66 | 0.55 | 0.37 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 15 | 0.64 | 0.28 | 0.61 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 15 | 0.48 | 0.21 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 15 | 0.48 | 0.21 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 15 | 0.48 | 0.21 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 15 | 0.48 | 0.21 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 15 | 0.48 | 0.21 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 15 | 0.48 | 0.21 | 0.48 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 15 | 0.41 | 0.17 | 0.46 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 15 | 0.41 | 0.17 | 0.46 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 15 | 0.38 | 0.15 | 0.34 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 15 | 0.32 | 0.11 | 0.36 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 15 | 0.32 | 0.11 | 0.36 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 15 | 0.32 | 0.11 | 0.36 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 15 | 0.25 | 0.1 | 0.22 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 15 | 0.25 | 0.1 | 0.22 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 15 | 0.25 | 0.1 | 0.22 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 15 | 0.2 | 0.06 | 0.19 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 15 | 0.2 | 0.06 | 0.19 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 15 | 0.2 | 0.06 | 0.19 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 14 | 1.71 | 1.48 | 1.3 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 14 | 1.54 | 0.38 | 1.46 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 14 | 1.54 | 0.38 | 1.46 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 14 | 1.54 | 0.38 | 1.46 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 14 | 1.09 | 0.65 | 0.9 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 14 | 1.09 | 0.65 | 0.9 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 14 | 1.05 | 0.71 | 1.03 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 14 | 0.92 | 0.61 | 0.73 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 14 | 0.8 | 0.54 | 0.78 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 14 | 0.8 | 0.54 | 0.78 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 14 | 0.8 | 0.54 | 0.78 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 14 | 0.75 | 0.37 | 0.74 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 14 | 0.73 | 0.64 | 0.59 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 14 | 0.73 | 0.64 | 0.59 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 14 | 0.73 | 0.64 | 0.59 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 14 | 0.73 | 0.64 | 0.59 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 14 | 0.73 | 0.64 | 0.59 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 14 | 0.73 | 0.64 | 0.59 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 14 | 0.61 | 0.39 | 0.44 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 14 | 0.61 | 0.39 | 0.44 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 14 | 0.61 | 0.39 | 0.44 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 14 | 0.6 | 0.43 | 0.36 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 14 | 0.6 | 0.43 | 0.36 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 14 | 0.6 | 0.43 | 0.36 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 14 | 0.43 | 0.18 | 0.4 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 14 | 0.43 | 0.18 | 0.4 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 14 | 0.43 | 0.18 | 0.4 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 14 | 0.43 | 0.14 | 0.37 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 14 | 0.39 | 0.14 | 0.38 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 14 | 0.38 | 0.09 | 0.38 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 14 | 0.29 | 0.13 | 0.28 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 14 | 0.29 | 0.13 | 0.28 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 14 | 0.29 | 0.13 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 14 | 0.28 | 0.16 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 14 | 0.22 | 0.05 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 14 | 0.22 | 0.05 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 14 | 0.22 | 0.05 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 14 | 0.22 | 0.05 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 14 | 0.22 | 0.05 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 14 | 0.22 | 0.05 | 0.24 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 13 | 2.62 | 1.09 | 2.94 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 13 | 2.38 | 1.14 | 2.65 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 13 | 1.73 | 0.49 | 1.86 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 13 | 1.73 | 0.49 | 1.86 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 13 | 1.73 | 0.49 | 1.86 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 13 | 1.66 | 1.05 | 1.35 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 13 | 1.15 | 0.7 | 1.05 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 13 | 1.07 | 1.11 | 0.43 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 13 | 1.06 | 0.59 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 13 | 1.06 | 0.59 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 13 | 1.06 | 0.59 | 1.11 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 13 | 0.87 | 0.61 | 0.9 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 13 | 0.81 | 0.51 | 0.58 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 13 | 0.78 | 0.42 | 0.84 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 13 | 0.74 | 0.35 | 0.8 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 13 | 0.74 | 0.35 | 0.8 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 13 | 0.74 | 0.35 | 0.8 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 13 | 0.72 | 0.37 | 0.73 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 13 | 0.63 | 0.44 | 0.45 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 13 | 0.63 | 0.44 | 0.45 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 13 | 0.63 | 0.44 | 0.45 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 13 | 0.62 | 0.37 | 0.48 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 13 | 0.62 | 0.37 | 0.48 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 13 | 0.62 | 0.37 | 0.48 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 13 | 0.55 | 0.15 | 0.56 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 13 | 0.48 | 0.12 | 0.48 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 13 | 0.46 | 0.23 | 0.39 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 13 | 0.46 | 0.23 | 0.39 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 13 | 0.46 | 0.23 | 0.39 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 13 | 0.44 | 0.24 | 0.39 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 13 | 0.44 | 0.24 | 0.39 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 13 | 0.43 | 0.32 | 0.4 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 13 | 0.43 | 0.32 | 0.4 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 13 | 0.43 | 0.23 | 0.39 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 13 | 0.43 | 0.23 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 13 | 0.43 | 0.23 | 0.39 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 13 | 0.42 | 0.2 | 0.43 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 13 | 0.42 | 0.2 | 0.43 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 13 | 0.42 | 0.2 | 0.43 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 13 | 0.42 | 0.14 | 0.41 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 13 | 0.4 | 0.17 | 0.36 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 13 | 0.4 | 0.28 | 0.27 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 13 | 0.38 | 0.21 | 0.3 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 13 | 0.34 | 0.18 | 0.34 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 13 | 0.34 | 0.18 | 0.34 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 13 | 0.15 | 0.02 | 0.15 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 13 | 0.15 | 0.02 | 0.15 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 13 | 0.15 | 0.02 | 0.15 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 12 | 3.0 | 0.22 | 2.98 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 12 | 3.0 | 0.22 | 2.98 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 12 | 3.0 | 0.22 | 2.98 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 12 | 2.42 | 0.19 | 2.43 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 12 | 2.36 | 0.69 | 2.13 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 12 | 2.07 | 1.42 | 1.51 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 12 | 2.07 | 0.56 | 2.16 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 12 | 1.82 | 1.14 | 1.68 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 12 | 1.82 | 1.14 | 1.68 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 12 | 1.82 | 1.14 | 1.68 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 12 | 1.75 | 0.65 | 1.62 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 12 | 1.75 | 0.65 | 1.62 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 12 | 1.5 | 0.48 | 1.37 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 12 | 1.4 | 0.13 | 1.4 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 12 | 1.35 | 0.66 | 1.33 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 12 | 1.23 | 0.69 | 1.27 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 12 | 1.23 | 0.69 | 1.27 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 12 | 1.23 | 0.69 | 1.27 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 12 | 1.18 | 0.04 | 1.17 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 12 | 1.1 | 0.69 | 1.11 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 12 | 1.1 | 0.69 | 1.11 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 12 | 1.1 | 0.69 | 1.11 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 12 | 1.07 | 0.99 | 0.5 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 12 | 1.07 | 0.99 | 0.5 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 12 | 0.94 | 0.21 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 12 | 0.94 | 0.21 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 12 | 0.94 | 0.21 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 12 | 0.94 | 0.21 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 12 | 0.94 | 0.21 | 0.91 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 12 | 0.94 | 0.21 | 0.91 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 12 | 0.93 | 0.64 | 0.73 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 12 | 0.85 | 0.07 | 0.86 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 12 | 0.85 | 0.07 | 0.86 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 12 | 0.82 | 0.38 | 0.78 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 12 | 0.82 | 0.38 | 0.78 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 12 | 0.81 | 0.07 | 0.78 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 12 | 0.72 | 0.47 | 0.6 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 12 | 0.71 | 0.36 | 0.72 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 12 | 0.71 | 0.44 | 0.7 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 12 | 0.71 | 0.44 | 0.7 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 12 | 0.71 | 0.44 | 0.7 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 12 | 0.68 | 0.62 | 0.52 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 12 | 0.61 | 0.39 | 0.53 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 12 | 0.61 | 0.46 | 0.46 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 12 | 0.61 | 0.46 | 0.46 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 12 | 0.51 | 0.3 | 0.48 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 12 | 0.44 | 0.24 | 0.44 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 12 | 0.39 | 0.22 | 0.36 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 12 | 0.39 | 0.22 | 0.36 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 12 | 0.39 | 0.22 | 0.36 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 12 | 0.38 | 0.17 | 0.4 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 12 | 0.38 | 0.17 | 0.4 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 12 | 0.38 | 0.17 | 0.4 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 12 | 0.38 | 0.2 | 0.3 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 12 | 0.38 | 0.2 | 0.3 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 12 | 0.22 | 0.1 | 0.2 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 12 | 0.22 | 0.09 | 0.2 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 12 | 0.2 | 0.08 | 0.18 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 12 | 0.2 | 0.08 | 0.18 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 11 | 1.26 | 0.71 | 1.29 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 11 | 1.26 | 0.71 | 1.29 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 11 | 1.26 | 0.71 | 1.29 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 11 | 1.07 | 0.76 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 11 | 1.07 | 0.76 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 11 | 1.07 | 0.76 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 11 | 1.07 | 0.76 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 11 | 1.07 | 0.76 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 11 | 1.07 | 0.76 | 0.93 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 11 | 0.94 | 0.55 | 1.01 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 11 | 0.94 | 0.55 | 1.01 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 11 | 0.94 | 0.55 | 1.01 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 11 | 0.94 | 0.55 | 1.01 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 11 | 0.92 | 0.61 | 0.69 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 11 | 0.92 | 0.61 | 0.69 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 11 | 0.92 | 0.61 | 0.69 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 11 | 0.92 | 0.61 | 0.69 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 11 | 0.89 | 0.71 | 0.87 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 11 | 0.89 | 0.71 | 0.87 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 11 | 0.89 | 0.71 | 0.87 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 11 | 0.72 | 0.36 | 0.68 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 11 | 0.72 | 0.36 | 0.68 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 11 | 0.71 | 0.69 | 0.32 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 11 | 0.67 | 0.42 | 0.67 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 11 | 0.67 | 0.42 | 0.67 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 11 | 0.67 | 0.42 | 0.67 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 11 | 0.6 | 0.32 | 0.57 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 11 | 0.58 | 0.16 | 0.56 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 11 | 0.43 | 0.12 | 0.44 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 11 | 0.42 | 0.19 | 0.41 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 11 | 0.42 | 0.19 | 0.41 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 11 | 0.42 | 0.19 | 0.41 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 11 | 0.41 | 0.17 | 0.41 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 11 | 0.35 | 0.15 | 0.35 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 11 | 0.31 | 0.16 | 0.24 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 11 | 0.3 | 0.13 | 0.26 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 11 | 0.27 | 0.22 | 0.21 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 11 | 0.26 | 0.11 | 0.23 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 11 | 0.24 | 0.07 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 11 | 0.24 | 0.07 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 11 | 0.24 | 0.07 | 0.24 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 11 | 0.23 | 0.07 | 0.23 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 11 | 0.22 | 0.12 | 0.16 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 11 | 0.22 | 0.12 | 0.16 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 11 | 0.22 | 0.12 | 0.16 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 11 | 0.2 | 0.05 | 0.19 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 10 | 2.07 | 1.39 | 2.5 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 10 | 2.07 | 1.39 | 2.5 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 10 | 1.67 | 0.94 | 1.86 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 10 | 1.67 | 0.94 | 1.86 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 10 | 1.67 | 0.94 | 1.86 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 10 | 1.65 | 1.18 | 1.74 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 10 | 1.65 | 1.18 | 1.74 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 10 | 1.65 | 1.18 | 1.74 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 10 | 0.97 | 0.29 | 0.94 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 10 | 0.86 | 0.43 | 0.76 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 10 | 0.86 | 0.43 | 0.76 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 10 | 0.8 | 0.41 | 0.68 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 10 | 0.8 | 0.41 | 0.68 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 10 | 0.8 | 0.41 | 0.68 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 10 | 0.8 | 0.41 | 0.68 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 10 | 0.79 | 0.7 | 0.42 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 10 | 0.78 | 0.45 | 0.66 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 10 | 0.76 | 0.72 | 0.47 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 10 | 0.76 | 0.44 | 0.74 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 10 | 0.76 | 0.44 | 0.74 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 10 | 0.74 | 0.44 | 0.64 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 10 | 0.59 | 0.29 | 0.55 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 10 | 0.52 | 0.3 | 0.46 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 10 | 0.52 | 0.2 | 0.54 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 10 | 0.52 | 0.2 | 0.54 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 10 | 0.52 | 0.2 | 0.54 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 10 | 0.51 | 0.31 | 0.42 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 10 | 0.48 | 0.55 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 10 | 0.48 | 0.55 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 10 | 0.48 | 0.55 | 0.22 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 10 | 0.47 | 0.22 | 0.48 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 10 | 0.46 | 0.22 | 0.52 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 10 | 0.46 | 0.22 | 0.52 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 10 | 0.45 | 0.36 | 0.28 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 10 | 0.45 | 0.43 | 0.29 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 10 | 0.45 | 0.43 | 0.29 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 10 | 0.45 | 0.43 | 0.29 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 10 | 0.44 | 0.34 | 0.24 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 10 | 0.44 | 0.34 | 0.24 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 10 | 0.44 | 0.34 | 0.24 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 10 | 0.44 | 0.18 | 0.42 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 10 | 0.38 | 0.16 | 0.32 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 10 | 0.37 | 0.24 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 10 | 0.35 | 0.22 | 0.26 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 10 | 0.33 | 0.13 | 0.32 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 10 | 0.33 | 0.13 | 0.32 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 10 | 0.33 | 0.13 | 0.32 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 10 | 0.3 | 0.11 | 0.3 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 10 | 0.3 | 0.08 | 0.32 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 10 | 0.28 | 0.14 | 0.24 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 10 | 0.28 | 0.14 | 0.24 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 10 | 0.28 | 0.14 | 0.24 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 10 | 0.18 | 0.05 | 0.22 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 10 | 0.18 | 0.06 | 0.17 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 10 | 0.15 | 0.04 | 0.14 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 9 | 1.3 | 0.56 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 9 | 1.3 | 0.56 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 9 | 1.3 | 0.56 | 1.15 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 9 | 1.25 | 0.6 | 1.32 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 9 | 1.17 | 0.85 | 1.35 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 9 | 1.17 | 0.85 | 1.35 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 9 | 1.15 | 0.44 | 1.16 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 9 | 0.92 | 0.51 | 1.07 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 9 | 0.91 | 0.72 | 0.65 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 9 | 0.91 | 0.72 | 0.65 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 9 | 0.91 | 0.72 | 0.65 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 9 | 0.91 | 0.44 | 0.87 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 9 | 0.91 | 0.44 | 0.87 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 9 | 0.91 | 0.44 | 0.87 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 9 | 0.8 | 0.61 | 0.41 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 9 | 0.78 | 0.69 | 0.52 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 9 | 0.71 | 0.31 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 9 | 0.71 | 0.31 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 9 | 0.71 | 0.31 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 9 | 0.71 | 0.31 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 9 | 0.71 | 0.31 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 9 | 0.71 | 0.31 | 0.73 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 9 | 0.63 | 0.19 | 0.66 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 9 | 0.47 | 0.17 | 0.48 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 9 | 0.47 | 0.17 | 0.48 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 9 | 0.47 | 0.17 | 0.48 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 9 | 0.45 | 0.35 | 0.28 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 9 | 0.45 | 0.35 | 0.28 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 9 | 0.4 | 0.11 | 0.46 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 9 | 0.33 | 0.16 | 0.28 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 9 | 0.33 | 0.16 | 0.28 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 9 | 0.33 | 0.16 | 0.28 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 9 | 0.28 | 0.07 | 0.3 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 9 | 0.23 | 0.07 | 0.26 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 9 | 0.22 | 0.06 | 0.2 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 9 | 0.14 | 0.02 | 0.13 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 9 | 0.14 | 0.02 | 0.13 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 9 | 0.14 | 0.02 | 0.13 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 8 | 2.43 | 1.91 | 2.55 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 8 | 1.82 | 0.36 | 1.82 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 8 | 1.3 | 0.65 | 1.36 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 8 | 1.3 | 0.65 | 1.36 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 8 | 1.3 | 0.65 | 1.36 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 8 | 1.3 | 0.65 | 1.36 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 8 | 1.3 | 0.65 | 1.36 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 8 | 1.3 | 0.65 | 1.36 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 8 | 1.25 | 1.05 | 0.77 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 8 | 1.25 | 1.05 | 0.77 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 8 | 1.25 | 1.05 | 0.77 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 8 | 1.21 | 0.31 | 1.18 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 8 | 1.21 | 0.31 | 1.18 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 8 | 1.12 | 0.69 | 1.13 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 8 | 1.12 | 0.69 | 1.13 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 8 | 0.85 | 0.67 | 0.5 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 8 | 0.85 | 0.67 | 0.5 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 8 | 0.84 | 0.48 | 0.73 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 8 | 0.84 | 0.48 | 0.73 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 8 | 0.84 | 0.48 | 0.73 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 8 | 0.84 | 0.48 | 0.73 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 8 | 0.83 | 0.56 | 0.84 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 8 | 0.82 | 0.83 | 0.55 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 8 | 0.82 | 0.83 | 0.55 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 8 | 0.82 | 0.83 | 0.55 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 8 | 0.82 | 0.45 | 0.66 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 8 | 0.82 | 0.45 | 0.66 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 8 | 0.82 | 0.45 | 0.66 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 8 | 0.82 | 0.45 | 0.66 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 8 | 0.8 | 0.66 | 0.52 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 8 | 0.79 | 0.39 | 0.94 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 8 | 0.79 | 0.39 | 0.94 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 8 | 0.79 | 0.39 | 0.94 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 8 | 0.68 | 0.23 | 0.7 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 8 | 0.67 | 0.4 | 0.65 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 8 | 0.6 | 0.49 | 0.42 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 8 | 0.58 | 0.26 | 0.58 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 8 | 0.58 | 0.26 | 0.58 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 8 | 0.58 | 0.26 | 0.58 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 8 | 0.58 | 0.21 | 0.58 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 8 | 0.54 | 0.17 | 0.5 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 8 | 0.54 | 0.17 | 0.5 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 8 | 0.54 | 0.17 | 0.5 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 8 | 0.5 | 0.23 | 0.54 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 8 | 0.5 | 0.23 | 0.54 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 8 | 0.5 | 0.23 | 0.54 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 8 | 0.5 | 0.23 | 0.54 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 8 | 0.5 | 0.23 | 0.54 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 8 | 0.5 | 0.23 | 0.54 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 8 | 0.38 | 0.16 | 0.43 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 8 | 0.38 | 0.16 | 0.43 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 8 | 0.33 | 0.13 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 8 | 0.33 | 0.13 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 8 | 0.33 | 0.13 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 8 | 0.33 | 0.13 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 8 | 0.33 | 0.13 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 8 | 0.33 | 0.13 | 0.3 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 8 | 0.3 | 0.1 | 0.32 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 8 | 0.3 | 0.1 | 0.32 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 8 | 0.29 | 0.11 | 0.29 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 8 | 0.29 | 0.11 | 0.29 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 8 | 0.25 | 0.07 | 0.24 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 8 | 0.22 | 0.07 | 0.2 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 8 | 0.18 | 0.07 | 0.14 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 8 | 0.16 | 0.09 | 0.12 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 8 | 0.16 | 0.04 | 0.16 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 8 | 0.14 | 0.03 | 0.13 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 7 | 2.72 | 1.08 | 2.95 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 7 | 1.56 | 0.65 | 1.77 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 7 | 1.56 | 0.65 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 7 | 1.56 | 0.65 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 7 | 1.56 | 0.65 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 7 | 1.56 | 0.65 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 7 | 1.56 | 0.65 | 1.77 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 7 | 0.9 | 0.42 | 0.99 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 7 | 0.71 | 0.46 | 0.68 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 7 | 0.63 | 0.41 | 0.55 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 7 | 0.62 | 0.31 | 0.61 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 7 | 0.58 | 0.32 | 0.59 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 7 | 0.58 | 0.32 | 0.59 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 7 | 0.58 | 0.32 | 0.59 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 7 | 0.58 | 0.22 | 0.55 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 7 | 0.55 | 0.27 | 0.46 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 7 | 0.54 | 0.58 | 0.22 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 7 | 0.54 | 0.58 | 0.22 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 7 | 0.54 | 0.58 | 0.22 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 7 | 0.53 | 0.79 | 0.2 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 7 | 0.53 | 0.79 | 0.2 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 7 | 0.53 | 0.79 | 0.2 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 7 | 0.49 | 0.22 | 0.42 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 7 | 0.49 | 0.22 | 0.42 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 7 | 0.45 | 0.39 | 0.27 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 7 | 0.45 | 0.39 | 0.27 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 7 | 0.45 | 0.39 | 0.27 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 7 | 0.38 | 0.19 | 0.29 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 7 | 0.33 | 0.14 | 0.28 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 7 | 0.33 | 0.19 | 0.26 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 7 | 0.33 | 0.19 | 0.26 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 7 | 0.33 | 0.19 | 0.26 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 7 | 0.32 | 0.13 | 0.28 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 7 | 0.32 | 0.19 | 0.26 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 7 | 0.28 | 0.14 | 0.23 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 7 | 0.28 | 0.14 | 0.23 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 7 | 0.28 | 0.14 | 0.23 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 7 | 0.28 | 0.05 | 0.3 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 7 | 0.27 | 0.11 | 0.23 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 7 | 0.25 | 0.07 | 0.26 |
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 7 | 0.25 | 0.09 | 0.25 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 7 | 0.25 | 0.09 | 0.25 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 7 | 0.25 | 0.09 | 0.25 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 7 | 0.17 | 0.07 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 7 | 0.17 | 0.07 | 0.12 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 7 | 0.17 | 0.07 | 0.12 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 7 | 0.15 | 0.01 | 0.15 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 7 | 0.14 | 0.03 | 0.14 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 7 | 0.13 | 0.02 | 0.13 |
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 7 | 0.13 | 0.03 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 7 | 0.13 | 0.03 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 7 | 0.13 | 0.03 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 7 | 0.13 | 0.03 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 7 | 0.13 | 0.03 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 7 | 0.13 | 0.03 | 0.12 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 7 | 0.11 | 0.0 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 7 | 0.11 | 0.0 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 7 | 0.11 | 0.0 | 0.11 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 6 | 1.35 | 0.72 | 1.13 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 6 | 1.35 | 0.72 | 1.13 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 6 | 1.35 | 0.72 | 1.13 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 6 | 1.35 | 0.72 | 1.13 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 6 | 1.35 | 0.72 | 1.13 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 6 | 1.35 | 0.72 | 1.13 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG11 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG12 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG13 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG21 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG22 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG23 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG11 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG12 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG13 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG21 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG22 | 6 | 1.29 | 0.81 | 1.12 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG23 | 6 | 1.29 | 0.81 | 1.12 |
| (1,545) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 6 | 0.98 | 0.67 | 0.82 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG2 | 6 | 0.95 | 0.48 | 0.84 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG3 | 6 | 0.95 | 0.48 | 0.84 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG2 | 6 | 0.95 | 0.48 | 0.84 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG3 | 6 | 0.95 | 0.48 | 0.84 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG2 | 6 | 0.95 | 0.48 | 0.84 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG3 | 6 | 0.95 | 0.48 | 0.84 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG11 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG12 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG13 | 6 | 0.85 | 0.67 | 0.52 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG21 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG22 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG23 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG11 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG12 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG13 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG21 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG22 | 6 | 0.85 | 0.67 | 0.52 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG23 | 6 | 0.85 | 0.67 | 0.52 |
| (1,92) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 6 | 0.83 | 0.58 | 0.66 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD21 | 6 | 0.79 | 0.37 | 0.78 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD22 | 6 | 0.79 | 0.37 | 0.78 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD23 | 6 | 0.79 | 0.37 | 0.78 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD21 | 6 | 0.73 | 0.39 | 0.75 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD22 | 6 | 0.73 | 0.39 | 0.75 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD23 | 6 | 0.73 | 0.39 | 0.75 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG21 | 6 | 0.7 | 0.33 | 0.76 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG22 | 6 | 0.7 | 0.33 | 0.76 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG23 | 6 | 0.7 | 0.33 | 0.76 |
| (1,1624) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 6 | 0.66 | 0.59 | 0.45 |
| (1,1624) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 6 | 0.66 | 0.59 | 0.45 |
| (1,417) | 1:90:A:MET:HE1 | 1:94:A:GLU:HG2 | 6 | 0.65 | 0.32 | 0.61 |
| (1,417) | 1:90:A:MET:HE2 | 1:94:A:GLU:HG2 | 6 | 0.65 | 0.32 | 0.61 |
| (1,417) | 1:90:A:MET:HE3 | 1:94:A:GLU:HG2 | 6 | 0.65 | 0.32 | 0.61 |
| (1,1475) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 6 | 0.65 | 0.49 | 0.47 |
| (1,1475) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 6 | 0.65 | 0.49 | 0.47 |
| (1,183) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 6 | 0.55 | 0.28 | 0.64 |
| (1,278) | 1:74:A:LEU:HD11 | 1:87:A:VAL:HB | 6 | 0.52 | 0.25 | 0.61 |
| (1,278) | 1:74:A:LEU:HD12 | 1:87:A:VAL:HB | 6 | 0.52 | 0.25 | 0.61 |
| (1,278) | 1:74:A:LEU:HD13 | 1:87:A:VAL:HB | 6 | 0.52 | 0.25 | 0.61 |
| (1,1199) | 1:80:A:ILE:HG21 | 1:105:A:ALA:H | 6 | 0.49 | 0.25 | 0.45 |
| (1,1199) | 1:80:A:ILE:HG22 | 1:105:A:ALA:H | 6 | 0.49 | 0.25 | 0.45 |
| (1,1199) | 1:80:A:ILE:HG23 | 1:105:A:ALA:H | 6 | 0.49 | 0.25 | 0.45 |
| (1,444) | 1:31:A:LEU:HG | 1:95:A:LYS:HB3 | 6 | 0.49 | 0.46 | 0.24 |
| (1,543) | 1:108:A:GLU:HA | 1:118:A:LYS:HG2 | 6 | 0.49 | 0.26 | 0.56 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG21 | 6 | 0.38 | 0.19 | 0.35 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG22 | 6 | 0.38 | 0.19 | 0.35 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG23 | 6 | 0.38 | 0.19 | 0.35 |
| (1,1575) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 6 | 0.36 | 0.19 | 0.29 |
| (1,1575) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 6 | 0.36 | 0.19 | 0.29 |
| (1,1575) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 6 | 0.36 | 0.19 | 0.29 |
| (1,1575) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 6 | 0.36 | 0.19 | 0.29 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1575) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 6 | 0.36 | 0.19 | 0.29 |
| (1,1575) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 6 | 0.36 | 0.19 | 0.29 |
| (1,192) | 1:59:A:GLN:HA | 1:61:A:ASP:H | 6 | 0.35 | 0.25 | 0.3 |
| (1,1619) | 1:103:A:GLN:HG2 | 1:104:A:LEU:H | 6 | 0.33 | 0.16 | 0.26 |
| (1,1619) | 1:103:A:GLN:HG3 | 1:104:A:LEU:H | 6 | 0.33 | 0.16 | 0.26 |
| (1,1308) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 6 | 0.33 | 0.2 | 0.26 |
| (1,343) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 6 | 0.31 | 0.16 | 0.3 |
| (1,952) | 1:67:A:GLY:H | 1:68:A:LYS:HB2 | 6 | 0.31 | 0.15 | 0.3 |
| (1,457) | 1:29:A:LYS:H | 1:97:A:LEU:HB2 | 6 | 0.29 | 0.19 | 0.17 |
| (1,481) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HA | 6 | 0.27 | 0.15 | 0.2 |
| (1,481) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HA | 6 | 0.27 | 0.15 | 0.2 |
| (1,481) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HA | 6 | 0.27 | 0.15 | 0.2 |
| (1,212) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 6 | 0.26 | 0.01 | 0.26 |
| (1,1197) | 1:100:A:ILE:HG21 | 1:105:A:ALA:H | 6 | 0.25 | 0.05 | 0.26 |
| (1,1197) | 1:100:A:ILE:HG22 | 1:105:A:ALA:H | 6 | 0.25 | 0.05 | 0.26 |
| (1,1197) | 1:100:A:ILE:HG23 | 1:105:A:ALA:H | 6 | 0.25 | 0.05 | 0.26 |
| (1,862) | 1:50:A:TYR:HB3 | 1:51:A:ASP:H | 6 | 0.25 | 0.08 | 0.24 |
| (1,482) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HB2 | 6 | 0.24 | 0.08 | 0.24 |
| (1,482) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HB2 | 6 | 0.24 | 0.08 | 0.24 |
| (1,482) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HB2 | 6 | 0.24 | 0.08 | 0.24 |
| (1,1204) | 1:100:A:ILE:HG21 | 1:106:A:TYR:H | 6 | 0.24 | 0.14 | 0.18 |
| (1,1204) | 1:100:A:ILE:HG22 | 1:106:A:TYR:H | 6 | 0.24 | 0.14 | 0.18 |
| (1,1204) | 1:100:A:ILE:HG23 | 1:106:A:TYR:H | 6 | 0.24 | 0.14 | 0.18 |
| (1,858) | 1:50:A:TYR:HD1 | 1:51:A:ASP:H | 6 | 0.24 | 0.05 | 0.23 |
| (1,1276) | 1:96:A:ALA:H | 1:127:A:LEU:H | 6 | 0.21 | 0.12 | 0.15 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB1 | 6 | 0.2 | 0.05 | 0.2 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB2 | 6 | 0.2 | 0.05 | 0.2 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB3 | 6 | 0.2 | 0.05 | 0.2 |
| (1,29) | 1:27:A:GLU:H | 1:27:A:GLU:HG2 | 6 | 0.19 | 0.04 | 0.18 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB1 | 6 | 0.16 | 0.04 | 0.16 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB2 | 6 | 0.16 | 0.04 | 0.16 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB3 | 6 | 0.16 | 0.04 | 0.16 |
| (1,1065) | 1:79:A:VAL:HG21 | 1:85:A:GLN:H | 6 | 0.16 | 0.07 | 0.12 |
| (1,1065) | 1:79:A:VAL:HG22 | 1:85:A:GLN:H | 6 | 0.16 | 0.07 | 0.12 |
| (1,1065) | 1:79:A:VAL:HG23 | 1:85:A:GLN:H | 6 | 0.16 | 0.07 | 0.12 |
| (1,530) | 1:106:A:TYR:HB3 | 1:111:A:TYR:HD2 | 5 | 1.79 | 1.0 | 2.07 |
| (1,226) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 5 | 1.33 | 0.55 | 1.37 |
| (1,1299) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 5 | 1.23 | 0.34 | 1.3 |
| (1,1299) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 5 | 1.23 | 0.34 | 1.3 |
| (1,1299) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 5 | 1.23 | 0.34 | 1.3 |
| (1,896) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 5 | 0.83 | 0.66 | 0.69 |
| (1,403) | 1:89:A:THR:HG21 | 1:98:A:PHE:HD2 | 5 | 0.71 | 0.16 | 0.74 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,403) | 1:89:A:THR:HG22 | 1:98:A:PHE:HD2 | 5 | 0.71 | 0.16 | 0.74 |
| (1,403) | 1:89:A:THR:HG23 | 1:98:A:PHE:HD2 | 5 | 0.71 | 0.16 | 0.74 |
| (1,689) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD1 | 5 | 0.66 | 0.09 | 0.68 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 5 | 0.55 | 0.21 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 5 | 0.55 | 0.21 | 0.52 |
| (1,449) | 1:32:A:THR:HB | 1:95:A:LYS:HE2 | 5 | 0.54 | 0.32 | 0.49 |
| (1,528) | 1:80:A:ILE:HG21 | 1:106:A:TYR:HA | 5 | 0.49 | 0.49 | 0.28 |
| (1,528) | 1:80:A:ILE:HG22 | 1:106:A:TYR:HA | 5 | 0.49 | 0.49 | 0.28 |
| (1,528) | 1:80:A:ILE:HG23 | 1:106:A:TYR:HA | 5 | 0.49 | 0.49 | 0.28 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG21 | 5 | 0.49 | 0.4 | 0.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG22 | 5 | 0.49 | 0.4 | 0.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG23 | 5 | 0.49 | 0.4 | 0.24 |
| (1,929) | 1:63:A:SER:H | 1:64:A:ARG:HG3 | 5 | 0.48 | 0.19 | 0.5 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG11 | 5 | 0.46 | 0.19 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG12 | 5 | 0.46 | 0.19 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG13 | 5 | 0.46 | 0.19 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG11 | 5 | 0.46 | 0.19 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG12 | 5 | 0.46 | 0.19 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG13 | 5 | 0.46 | 0.19 | 0.53 |
| (1,681) | 1:50:A:TYR:H | 1:50:A:TYR:HD2 | 5 | 0.43 | 0.36 | 0.29 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG21 | 5 | 0.39 | 0.08 | 0.39 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG22 | 5 | 0.39 | 0.08 | 0.39 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG23 | 5 | 0.39 | 0.08 | 0.39 |
| (1,910) | 1:55:A:PRO:HA | 1:57:A:GLY:H | 5 | 0.38 | 0.24 | 0.38 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB2 | 5 | 0.37 | 0.17 | 0.38 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB3 | 5 | 0.37 | 0.17 | 0.38 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1405) | 1:44:A:LYS:HE2 | 1:45:A:LYS:H | 5 | 0.36 | 0.14 | 0.3 |
| (1,1405) | 1:44:A:LYS:HE3 | 1:45:A:LYS:H | 5 | 0.36 | 0.14 | 0.3 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG21 | 5 | 0.35 | 0.11 | 0.35 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG22 | 5 | 0.35 | 0.11 | 0.35 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG23 | 5 | 0.35 | 0.11 | 0.35 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG2 | 5 | 0.33 | 0.08 | 0.3 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG3 | 5 | 0.33 | 0.08 | 0.3 |
| (1,972) | 1:70:A:PHE:HD2 | 1:71:A:GLN:H | 5 | 0.32 | 0.06 | 0.29 |
| (1,266) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 5 | 0.31 | 0.15 | 0.26 |
| (1,266) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 5 | 0.31 | 0.15 | 0.26 |
| (1,266) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 5 | 0.31 | 0.15 | 0.26 |
| (1,1441) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 5 | 0.24 | 0.09 | 0.25 |
| (1,1441) | 1:53:A:ARG:HD3 | 1:57:A:GLY:HA2 | 5 | 0.24 | 0.09 | 0.25 |
| (1,216) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 5 | 0.24 | 0.04 | 0.26 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD11 | 5 | 0.24 | 0.1 | 0.22 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD12 | 5 | 0.24 | 0.1 | 0.22 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD13 | 5 | 0.24 | 0.1 | 0.22 |
| (1,866) | 1:51:A:ASP:H | 1:124:A:GLU:HB3 | 5 | 0.23 | 0.12 | 0.2 |
| (1,1120) | 1:34:A:GLY:HA2 | 1:94:A:GLU:H | 5 | 0.22 | 0.1 | 0.18 |
| (1,775) | 1:34:A:GLY:H | 1:94:A:GLU:HB3 | 5 | 0.21 | 0.05 | 0.21 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB1 | 5 | 0.2 | 0.09 | 0.15 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB2 | 5 | 0.2 | 0.09 | 0.15 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB3 | 5 | 0.2 | 0.09 | 0.15 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 5 | 0.17 | 0.02 | 0.17 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB3 | 5 | 0.17 | 0.02 | 0.17 |
| (1,977) | 1:47:A:THR:HG21 | 1:71:A:GLN:H | 5 | 0.17 | 0.04 | 0.17 |
| (1,977) | 1:47:A:THR:HG22 | 1:71:A:GLN:H | 5 | 0.17 | 0.04 | 0.17 |
| (1,977) | 1:47:A:THR:HG23 | 1:71:A:GLN:H | 5 | 0.17 | 0.04 | 0.17 |
| (1,1218) | 1:111:A:TYR:H | 1:111:A:TYR:HB3 | 5 | 0.15 | 0.01 | 0.15 |
| (1,498) | 1:103:A:GLN:HA | 1:104:A:LEU:HG | 5 | 0.14 | 0.03 | 0.13 |
| (1,1173) | 1:102:A:TYR:H | 1:102:A:TYR:HE1 | 4 | 1.47 | 0.07 | 1.48 |
| (1,959) | 1:49:A:HIS:HD2 | 1:70:A:PHE:H | 4 | 1.31 | 0.38 | 1.43 |
| (1,902) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 4 | 1.17 | 0.88 | 1.01 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE1 | 4 | 1.0 | 0.1 | 0.98 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE2 | 4 | 1.0 | 0.1 | 0.98 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE3 | 4 | 1.0 | 0.1 | 0.98 |
| (1,395) | 1:40:A:PRO:HG2 | 1:88:A:ALA:HA | 4 | 0.99 | 0.79 | 0.89 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG2 | 4 | 0.88 | 0.54 | 0.8 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG3 | 4 | 0.88 | 0.54 | 0.8 |
| (1,800) | 1:41:A:GLN:H | 1:44:A:LYS:HB2 | 4 | 0.82 | 0.27 | 0.74 |
| (1,903) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 4 | 0.79 | 0.4 | 0.86 |
| (1,494) | 1:102:A:TYR:HB2 | 1:102:A:TYR:HE2 | 4 | 0.78 | 0.02 | 0.78 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,450) | 1:32:A:THR:HB | 1:95:A:LYS:HE3 | 4 | 0.68 | 0.32 | 0.7 |
| (1,651) | 1:92:A:LEU:HD11 | 1:129:A:ALA:HA | 4 | 0.66 | 0.19 | 0.6 |
| (1,651) | 1:92:A:LEU:HD12 | 1:129:A:ALA:HA | 4 | 0.66 | 0.19 | 0.6 |
| (1,651) | 1:92:A:LEU:HD13 | 1:129:A:ALA:HA | 4 | 0.66 | 0.19 | 0.6 |
| (1,106) | 1:45:A:LYS:H | 1:45:A:LYS:HE3 | 4 | 0.62 | 0.24 | 0.64 |
| (1,1025) | 1:82:A:GLY:H | 1:104:A:LEU:HA | 4 | 0.55 | 0.34 | 0.55 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG21 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG22 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG23 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG21 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG22 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG23 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG21 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG22 | 4 | 0.52 | 0.42 | 0.35 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG23 | 4 | 0.52 | 0.42 | 0.35 |
| (1,155) | 1:51:A:ASP:HB3 | 1:124:A:GLU:H | 4 | 0.5 | 0.18 | 0.42 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG21 | 4 | 0.48 | 0.32 | 0.42 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG22 | 4 | 0.48 | 0.32 | 0.42 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG23 | 4 | 0.48 | 0.32 | 0.42 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG21 | 4 | 0.44 | 0.16 | 0.53 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG22 | 4 | 0.44 | 0.16 | 0.53 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG23 | 4 | 0.44 | 0.16 | 0.53 |
| (1,145) | 1:49:A:HIS:HB2 | 1:126:A:GLU:HG2 | 4 | 0.42 | 0.09 | 0.4 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD11 | 4 | 0.38 | 0.04 | 0.4 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD12 | 4 | 0.38 | 0.04 | 0.4 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD13 | 4 | 0.38 | 0.04 | 0.4 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD21 | 4 | 0.38 | 0.04 | 0.4 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD22 | 4 | 0.38 | 0.04 | 0.4 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD23 | 4 | 0.38 | 0.04 | 0.4 |
| (1,153) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 4 | 0.38 | 0.16 | 0.38 |
| (1,1162) | 1:27:A:GLU:HB2 | 1:99:A:THR:H | 4 | 0.37 | 0.12 | 0.4 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG11 | 4 | 0.36 | 0.12 | 0.4 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG12 | 4 | 0.36 | 0.12 | 0.4 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG13 | 4 | 0.36 | 0.12 | 0.4 |
| (1,276) | 1:74:A:LEU:HD11 | 1:88:A:ALA:H | 4 | 0.36 | 0.29 | 0.24 |
| (1,276) | 1:74:A:LEU:HD12 | 1:88:A:ALA:H | 4 | 0.36 | 0.29 | 0.24 |
| (1,276) | 1:74:A:LEU:HD13 | 1:88:A:ALA:H | 4 | 0.36 | 0.29 | 0.24 |
| (1,966) | 1:69:A:PRO:HB3 | 1:70:A:PHE:H | 4 | 0.36 | 0.23 | 0.33 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB1 | 4 | 0.35 | 0.18 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB2 | 4 | 0.35 | 0.18 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB3 | 4 | 0.35 | 0.18 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB1 | 4 | 0.35 | 0.18 | 0.25 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB2 | 4 | 0.35 | 0.18 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB3 | 4 | 0.35 | 0.18 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB1 | 4 | 0.35 | 0.18 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB2 | 4 | 0.35 | 0.18 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB3 | 4 | 0.35 | 0.18 | 0.25 |
| (1,490) | 1:102:A:TYR:HB3 | 1:102:A:TYR:HE1 | 4 | 0.34 | 0.01 | 0.34 |
| (1,1105) | 1:38:A:THR:H | 1:92:A:LEU:H | 4 | 0.34 | 0.31 | 0.2 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG21 | 4 | 0.33 | 0.16 | 0.36 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG22 | 4 | 0.33 | 0.16 | 0.36 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG23 | 4 | 0.33 | 0.16 | 0.36 |
| (1,824) | 1:44:A:LYS:HB3 | 1:45:A:LYS:H | 4 | 0.3 | 0.1 | 0.32 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB1 | 4 | 0.3 | 0.05 | 0.31 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB2 | 4 | 0.3 | 0.05 | 0.31 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB3 | 4 | 0.3 | 0.05 | 0.31 |
| (1,797) | 1:41:A:GLN:H | 1:41:A:GLN:HG2 | 4 | 0.3 | 0.17 | 0.26 |
| (1,229) | 1:69:A:PRO:HA | 1:128:A:LEU:HG | 4 | 0.28 | 0.22 | 0.17 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD11 | 4 | 0.28 | 0.12 | 0.3 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD12 | 4 | 0.28 | 0.12 | 0.3 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD13 | 4 | 0.28 | 0.12 | 0.3 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG11 | 4 | 0.26 | 0.15 | 0.18 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG12 | 4 | 0.26 | 0.15 | 0.18 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG13 | 4 | 0.26 | 0.15 | 0.18 |
| (1,48) | 1:34:A:GLY:HA2 | 1:94:A:GLU:HB3 | 4 | 0.24 | 0.08 | 0.28 |
| (1,813) | 1:43:A:GLY:H | 1:74:A:LEU:HG | 4 | 0.23 | 0.11 | 0.21 |
| (1,425) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 4 | 0.21 | 0.06 | 0.22 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG11 | 4 | 0.2 | 0.07 | 0.18 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG12 | 4 | 0.2 | 0.07 | 0.18 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG13 | 4 | 0.2 | 0.07 | 0.18 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG21 | 4 | 0.2 | 0.05 | 0.22 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG22 | 4 | 0.2 | 0.05 | 0.22 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG23 | 4 | 0.2 | 0.05 | 0.22 |
| (1,1380) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 4 | 0.19 | 0.04 | 0.2 |
| (1,1380) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 4 | 0.19 | 0.04 | 0.2 |
| (1,378) | 1:81:A:LYS:HA | 1:84:A:ASP:HB3 | 4 | 0.19 | 0.07 | 0.19 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB1 | 4 | 0.19 | 0.05 | 0.17 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB2 | 4 | 0.19 | 0.05 | 0.17 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB3 | 4 | 0.19 | 0.05 | 0.17 |
| (1,220) | 1:66:A:ARG:HA | 1:66:A:ARG:HD2 | 4 | 0.18 | 0.07 | 0.16 |
| (1,812) | 1:43:A:GLY:H | 1:44:A:LYS:HB2 | 4 | 0.18 | 0.06 | 0.16 |
| (1,160) | 1:53:A:ARG:HB2 | 1:59:A:GLN:HA | 4 | 0.16 | 0.01 | 0.16 |
| (1,603) | 1:123:A:PHE:H | 1:124:A:GLU:HA | 4 | 0.15 | 0.03 | 0.16 |
| (1,887) | 1:53:A:ARG:HB3 | 1:54:A:PHE:H | 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) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,328) | 1:80:A:ILE:HG13 | 1:83:A:TRP:H | 4 | 0.13 | 0.01 | 0.12 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD2 | 4 | 0.13 | 0.03 | 0.12 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD3 | 4 | 0.13 | 0.03 | 0.12 |
| (1,836) | 1:47:A:THR:H | 1:128:A:LEU:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,1284) | 1:127:A:LEU:H | 1:127:A:LEU:HG | 4 | 0.12 | 0.0 | 0.12 |
| (1,1600) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG2 | 3 | 2.03 | 0.11 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG2 | 3 | 2.03 | 0.11 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG2 | 3 | 2.03 | 0.11 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG2 | 3 | 2.03 | 0.11 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG2 | 3 | 2.03 | 0.11 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG2 | 3 | 2.03 | 0.11 | 1.95 |
| (1,609) | 1:123:A:PHE:HA | 1:124:A:GLU:HG3 | 3 | 1.2 | 0.09 | 1.15 |
| (1,534) | 1:106:A:TYR:HB2 | 1:111:A:TYR:HD2 | 3 | 1.03 | 0.52 | 1.34 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB1 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB2 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB3 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB1 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB2 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB3 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB1 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB2 | 3 | 0.98 | 0.37 | 1.08 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB3 | 3 | 0.98 | 0.37 | 1.08 |
| (1,587) | 1:115:A:ILE:HD11 | 1:121:A:LEU:HG | 3 | 0.78 | 0.22 | 0.67 |
| (1,587) | 1:115:A:ILE:HD12 | 1:121:A:LEU:HG | 3 | 0.78 | 0.22 | 0.67 |
| (1,587) | 1:115:A:ILE:HD13 | 1:121:A:LEU:HG | 3 | 0.78 | 0.22 | 0.67 |
| (1,1130) | 1:90:A:MET:HE1 | 1:95:A:LYS:H | 3 | 0.75 | 0.29 | 0.79 |
| (1,1130) | 1:90:A:MET:HE2 | 1:95:A:LYS:H | 3 | 0.75 | 0.29 | 0.79 |
| (1,1130) | 1:90:A:MET:HE3 | 1:95:A:LYS:H | 3 | 0.75 | 0.29 | 0.79 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG11 | 3 | 0.69 | 0.2 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG12 | 3 | 0.69 | 0.2 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG13 | 3 | 0.69 | 0.2 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG21 | 3 | 0.69 | 0.2 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG22 | 3 | 0.69 | 0.2 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG23 | 3 | 0.69 | 0.2 | 0.83 |
| (1,371) | 1:81:A:LYS:HD3 | 1:84:A:ASP:HB2 | 3 | 0.64 | 0.46 | 0.4 |
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 3 | 0.6 | 0.04 | 0.59 |
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 3 | 0.6 | 0.04 | 0.59 |
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 3 | 0.6 | 0.04 | 0.59 |
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 3 | 0.6 | 0.04 | 0.59 |
| (1,292) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HG2 | 3 | 0.52 | 0.22 | 0.6 |
| (1,292) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HG2 | 3 | 0.52 | 0.22 | 0.6 |
| (1,292) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HG2 | 3 | 0.52 | 0.22 | 0.6 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD21 | 3 | 0.52 | 0.37 | 0.38 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD22 | 3 | 0.52 | 0.37 | 0.38 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD23 | 3 | 0.52 | 0.37 | 0.38 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB1 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB2 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB3 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB1 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB2 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB3 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB1 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB2 | 3 | 0.5 | 0.33 | 0.31 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB3 | 3 | 0.5 | 0.33 | 0.31 |
| (1,394) | 1:74:A:LEU:HD11 | 1:88:A:ALA:HA | 3 | 0.49 | 0.25 | 0.53 |
| (1,394) | 1:74:A:LEU:HD12 | 1:88:A:ALA:HA | 3 | 0.49 | 0.25 | 0.53 |
| (1,394) | 1:74:A:LEU:HD13 | 1:88:A:ALA:HA | 3 | 0.49 | 0.25 | 0.53 |
| (1,983) | 1:73:A:THR:H | 1:78:A:GLU:HB2 | 3 | 0.47 | 0.34 | 0.27 |
| (1,421) | 1:91:A:THR:HA | 1:127:A:LEU:HG | 3 | 0.46 | 0.23 | 0.32 |
| (1,93) | 1:41:A:GLN:HG3 | 1:44:A:LYS:HG2 | 3 | 0.45 | 0.36 | 0.27 |
| (1,1265) | 1:124:A:GLU:HB3 | 1:125:A:VAL:H | 3 | 0.44 | 0.05 | 0.46 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD11 | 3 | 0.4 | 0.19 | 0.29 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD12 | 3 | 0.4 | 0.19 | 0.29 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD13 | 3 | 0.4 | 0.19 | 0.29 |
| (1,623) | 1:95:A:LYS:HB2 | 1:126:A:GLU:HA | 3 | 0.39 | 0.13 | 0.39 |
| (1,802) | 1:41:A:GLN:H | 1:74:A:LEU:HB3 | 3 | 0.37 | 0.28 | 0.21 |
| (1,1584) | 1:95:A:LYS:HG2 | 1:124:A:GLU:HB3 | 3 | 0.36 | 0.14 | 0.43 |
| (1,1584) | 1:95:A:LYS:HG3 | 1:124:A:GLU:HB3 | 3 | 0.36 | 0.14 | 0.43 |
| (1,608) | 1:97:A:LEU:HG | 1:124:A:GLU:HG3 | 3 | 0.35 | 0.14 | 0.36 |
| (1,950) | 1:64:A:ARG:HA | 1:67:A:GLY:H | 3 | 0.34 | 0.12 | 0.39 |
| (1,749) | 1:27:A:GLU:H | 1:27:A:GLU:HG3 | 3 | 0.33 | 0.05 | 0.31 |
| (1,1281) | 1:95:A:LYS:HB2 | 1:127:A:LEU:H | 3 | 0.32 | 0.13 | 0.38 |
| (1,161) | 1:53:A:ARG:HA | 1:60:A:PHE:H | 3 | 0.28 | 0.14 | 0.28 |
| (1,1029) | 1:82:A:GLY:H | 1:104:A:LEU:HB3 | 3 | 0.26 | 0.1 | 0.21 |
| (1,1215) | 1:110:A:GLY:HA3 | 1:111:A:TYR:H | 3 | 0.26 | 0.02 | 0.27 |
| (1,1036) | 1:79:A:VAL:HB | 1:83:A:TRP:H | 3 | 0.24 | 0.08 | 0.24 |
| (1,520) | 1:100:A:ILE:HG21 | 1:105:A:ALA:HA | 3 | 0.23 | 0.09 | 0.29 |
| (1,520) | 1:100:A:ILE:HG22 | 1:105:A:ALA:HA | 3 | 0.23 | 0.09 | 0.29 |
| (1,520) | 1:100:A:ILE:HG23 | 1:105:A:ALA:HA | 3 | 0.23 | 0.09 | 0.29 |
| (1,541) | 1:108:A:GLU:HA | 1:118:A:LYS:HA | 3 | 0.23 | 0.04 | 0.22 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG21 | 3 | 0.23 | 0.04 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG22 | 3 | 0.23 | 0.04 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG23 | 3 | 0.23 | 0.04 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG21 | 3 | 0.23 | 0.04 | 0.24 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG22 | 3 | 0.23 | 0.04 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG23 | 3 | 0.23 | 0.04 | 0.24 |
| (1,227) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 3 | 0.21 | 0.07 | 0.23 |
| (1,1093) | 1:87:A:VAL:HG11 | 1:90:A:MET:H | 3 | 0.21 | 0.04 | 0.18 |
| (1,1093) | 1:87:A:VAL:HG12 | 1:90:A:MET:H | 3 | 0.21 | 0.04 | 0.18 |
| (1,1093) | 1:87:A:VAL:HG13 | 1:90:A:MET:H | 3 | 0.21 | 0.04 | 0.18 |
| (1,309) | 1:80:A:ILE:HA | 1:81:A:LYS:HB2 | 3 | 0.2 | 0.06 | 0.22 |
| (1,72) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 3 | 0.2 | 0.07 | 0.17 |
| (1,109) | 1:46:A:VAL:HB | 1:129:A:ALA:H | 3 | 0.19 | 0.1 | 0.12 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD11 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD12 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD13 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD11 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD12 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD13 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD11 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD12 | 3 | 0.19 | 0.07 | 0.14 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD13 | 3 | 0.19 | 0.07 | 0.14 |
| (1,1005) | 1:77:A:GLY:H | 1:78:A:GLU:H | 3 | 0.18 | 0.02 | 0.17 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG2 | 3 | 0.17 | 0.01 | 0.18 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG3 | 3 | 0.17 | 0.01 | 0.18 |
| (1,470) | 1:100:A:ILE:HB | 1:121:A:LEU:HB2 | 3 | 0.16 | 0.04 | 0.14 |
| (1,123) | 1:46:A:VAL:HG11 | 1:130:A:VAL:HB | 3 | 0.16 | 0.03 | 0.17 |
| (1,123) | 1:46:A:VAL:HG12 | 1:130:A:VAL:HB | 3 | 0.16 | 0.03 | 0.17 |
| (1,123) | 1:46:A:VAL:HG13 | 1:130:A:VAL:HB | 3 | 0.16 | 0.03 | 0.17 |
| (1,1037) | 1:80:A:ILE:HG12 | 1:83:A:TRP:H | 3 | 0.15 | 0.03 | 0.15 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG11 | 3 | 0.15 | 0.05 | 0.13 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG12 | 3 | 0.15 | 0.05 | 0.13 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG13 | 3 | 0.15 | 0.05 | 0.13 |
| (1,355) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA2 | 3 | 0.15 | 0.03 | 0.15 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB1 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB2 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB3 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB1 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB2 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB3 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB1 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB2 | 3 | 0.15 | 0.04 | 0.17 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB3 | 3 | 0.15 | 0.04 | 0.17 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 3 | 0.13 | 0.02 | 0.13 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 3 | 0.13 | 0.02 | 0.13 |
| (1,199) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 2 | 1.36 | 0.5 | 1.36 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,163) | 1:53:A:ARG:HG3 | 1:59:A:GLN:H | 2 | 1.03 | 0.84 | 1.03 |
| (1,393) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HA | 2 | 0.98 | 0.1 | 0.98 |
| (1,393) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HA | 2 | 0.98 | 0.1 | 0.98 |
| (1,393) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HA | 2 | 0.98 | 0.1 | 0.98 |
| (1,1064) | 1:81:A:LYS:HD3 | 1:85:A:GLN:H | 2 | 0.98 | 0.04 | 0.98 |
| (1,522) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HA | 2 | 0.94 | 0.53 | 0.94 |
| (1,522) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HA | 2 | 0.94 | 0.53 | 0.94 |
| (1,522) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HA | 2 | 0.94 | 0.53 | 0.94 |
| (1,705) | 1:49:A:HIS:HE1 | 1:64:A:ARG:HA | 2 | 0.9 | 0.68 | 0.9 |
| (1,94) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG3 | 2 | 0.88 | 0.66 | 0.88 |
| (1,462) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 2 | 0.87 | 0.64 | 0.87 |
| (1,462) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 2 | 0.87 | 0.64 | 0.87 |
| (1,462) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 2 | 0.87 | 0.64 | 0.87 |
| (1,39) | 1:32:A:THR:HB | 1:95:A:LYS:HB2 | 2 | 0.7 | 0.36 | 0.7 |
| (1,271) | 1:74:A:LEU:HD21 | 1:88:A:ALA:H | 2 | 0.57 | 0.02 | 0.57 |
| (1,271) | 1:74:A:LEU:HD22 | 1:88:A:ALA:H | 2 | 0.57 | 0.02 | 0.57 |
| (1,271) | 1:74:A:LEU:HD23 | 1:88:A:ALA:H | 2 | 0.57 | 0.02 | 0.57 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG21 | 2 | 0.57 | 0.23 | 0.57 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG22 | 2 | 0.57 | 0.23 | 0.57 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG23 | 2 | 0.57 | 0.23 | 0.57 |
| (1,200) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 2 | 0.56 | 0.05 | 0.56 |
| (1,1096) | 1:91:A:THR:H | 1:94:A:GLU:H | 2 | 0.55 | 0.22 | 0.55 |
| (1,1049) | 1:81:A:LYS:HD3 | 1:84:A:ASP:H | 2 | 0.54 | 0.06 | 0.54 |
| (1,575) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HG2 | 2 | 0.5 | 0.06 | 0.5 |
| (1,201) | 1:59:A:GLN:H | 1:59:A:GLN:HG3 | 2 | 0.49 | 0.06 | 0.49 |
| (1,644) | 1:49:A:HIS:HB2 | 1:128:A:LEU:HG | 2 | 0.47 | 0.16 | 0.47 |
| (1,1332) | 1:24:A:ALA:HA | 1:103:A:GLN:HG2 | 2 | 0.43 | 0.22 | 0.43 |
| (1,1332) | 1:24:A:ALA:HA | 1:103:A:GLN:HG3 | 2 | 0.43 | 0.22 | 0.43 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD11 | 2 | 0.41 | 0.18 | 0.41 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD12 | 2 | 0.41 | 0.18 | 0.41 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD13 | 2 | 0.41 | 0.18 | 0.41 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 2 | 0.4 | 0.1 | 0.4 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 2 | 0.4 | 0.1 | 0.4 |
| (1,354) | 1:82:A:GLY:HA2 | 1:104:A:LEU:HB3 | 2 | 0.4 | 0.16 | 0.4 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG21 | 2 | 0.39 | 0.24 | 0.39 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG22 | 2 | 0.39 | 0.24 | 0.39 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG23 | 2 | 0.39 | 0.24 | 0.39 |
| (1,1397) | 1:43:A:GLY:HA2 | 1:44:A:LYS:HG2 | 2 | 0.38 | 0.01 | 0.38 |
| (1,1397) | 1:43:A:GLY:HA2 | 1:44:A:LYS:HG3 | 2 | 0.38 | 0.01 | 0.38 |
| (1,1397) | 1:43:A:GLY:HA3 | 1:44:A:LYS:HG2 | 2 | 0.38 | 0.01 | 0.38 |
| (1,1397) | 1:43:A:GLY:HA3 | 1:44:A:LYS:HG3 | 2 | 0.38 | 0.01 | 0.38 |
| (1,38) | 1:31:A:LEU:HG | 1:32:A:THR:H | 2 | 0.36 | 0.1 | 0.36 |
| (1,443) | 1:32:A:THR:HG21 | 1:95:A:LYS:HB3 | 2 | 0.36 | 0.16 | 0.36 |
| (1,443) | 1:32:A:THR:HG22 | 1:95:A:LYS:HB3 | 2 | 0.36 | 0.16 | 0.36 |
| (1,443) | 1:32:A:THR:HG23 | 1:95:A:LYS:HB3 | 2 | 0.36 | 0.16 | 0.36 |
| (1,1470) | 1:59:A:GLN:H | 1:59:A:GLN:HG2 | 2 | 0.36 | 0.06 | 0.36 |
| (1,1470) | 1:59:A:GLN:H | 1:59:A:GLN:HG3 | 2 | 0.36 | 0.06 | 0.36 |
| (1,1314) | 1:13:A:GLU:H | 1:13:A:GLU:HB2 | 2 | 0.36 | 0.08 | 0.36 |
| (1,1314) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 2 | 0.36 | 0.08 | 0.36 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG11 | 2 | 0.35 | 0.07 | 0.35 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG12 | 2 | 0.35 | 0.07 | 0.35 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG13 | 2 | 0.35 | 0.07 | 0.35 |
| (1,232) | 1:48:A:VAL:H | 1:69:A:PRO:HB3 | 2 | 0.34 | 0.08 | 0.34 |
| (1,601) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB2 | 2 | 0.34 | 0.18 | 0.34 |
| (1,601) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB2 | 2 | 0.34 | 0.18 | 0.34 |
| (1,601) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB2 | 2 | 0.34 | 0.18 | 0.34 |
| (1,424) | 1:34:A:GLY:HA3 | 1:91:A:THR:HB | 2 | 0.33 | 0.0 | 0.33 |
| (1,228) | 1:47:A:THR:HG21 | 1:69:A:PRO:HA | 2 | 0.31 | 0.16 | 0.31 |
| (1,228) | 1:47:A:THR:HG22 | 1:69:A:PRO:HA | 2 | 0.31 | 0.16 | 0.31 |
| (1,228) | 1:47:A:THR:HG23 | 1:69:A:PRO:HA | 2 | 0.31 | 0.16 | 0.31 |
| (1,708) | 1:11:A:THR:HA | 1:12:A:LEU:H | 2 | 0.31 | 0.07 | 0.31 |
| (1,336) | 1:81:A:LYS:HB3 | 1:81:A:LYS:HE2 | 2 | 0.29 | 0.0 | 0.29 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB1 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB2 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB3 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB1 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB2 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB3 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB1 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB2 | 2 | 0.27 | 0.07 | 0.27 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB3 | 2 | 0.27 | 0.07 | 0.27 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG11 | 2 | 0.26 | 0.08 | 0.26 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG12 | 2 | 0.26 | 0.08 | 0.26 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG13 | 2 | 0.26 | 0.08 | 0.26 |
| (1,1213) | 1:109:A:ARG:HB3 | 1:110:A:GLY:H | 2 | 0.26 | 0.02 | 0.26 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG11 | 2 | 0.26 | 0.04 | 0.26 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG12 | 2 | 0.26 | 0.04 | 0.26 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG13 | 2 | 0.26 | 0.04 | 0.26 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG21 | 2 | 0.26 | 0.04 | 0.26 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG22 | 2 | 0.26 | 0.04 | 0.26 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG23 | 2 | 0.26 | 0.04 | 0.26 |
| (1,819) | 1:44:A:LYS:H | 1:44:A:LYS:HG2 | 2 | 0.26 | 0.05 | 0.26 |
| (1,391) | 1:46:A:VAL:HG21 | 1:87:A:VAL:HB | 2 | 0.26 | 0.02 | 0.26 |
| (1,391) | 1:46:A:VAL:HG22 | 1:87:A:VAL:HB | 2 | 0.26 | 0.02 | 0.26 |
| (1,391) | 1:46:A:VAL:HG23 | 1:87:A:VAL:HB | 2 | 0.26 | 0.02 | 0.26 |
| (1,700) | 1:79:A:VAL:HB | 1:83:A:TRP:HE3 | 2 | 0.25 | 0.08 | 0.25 |
| (1,965) | 1:69:A:PRO:HG3 | 1:70:A:PHE:H | 2 | 0.24 | 0.1 | 0.24 |
| (1,430) | 1:92:A:LEU:HD21 | 1:129:A:ALA:HA | 2 | 0.24 | 0.05 | 0.24 |
| (1,430) | 1:92:A:LEU:HD22 | 1:129:A:ALA:HA | 2 | 0.24 | 0.05 | 0.24 |
| (1,430) | 1:92:A:LEU:HD23 | 1:129:A:ALA:HA | 2 | 0.24 | 0.05 | 0.24 |
| (1,274) | 1:74:A:LEU:HD11 | 1:87:A:VAL:H | 2 | 0.23 | 0.12 | 0.23 |
| (1,274) | 1:74:A:LEU:HD12 | 1:87:A:VAL:H | 2 | 0.23 | 0.12 | 0.23 |
| (1,274) | 1:74:A:LEU:HD13 | 1:87:A:VAL:H | 2 | 0.23 | 0.12 | 0.23 |
| (1,1399) | 1:44:A:LYS:HB2 | 1:44:A:LYS:HE2 | 2 | 0.23 | 0.02 | 0.23 |
| (1,1399) | 1:44:A:LYS:HB2 | 1:44:A:LYS:HE3 | 2 | 0.23 | 0.02 | 0.23 |
| (1,147) | 1:50:A:TYR:HA | 1:124:A:GLU:HB3 | 2 | 0.22 | 0.04 | 0.22 |
| (1,690) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD2 | 2 | 0.22 | 0.07 | 0.22 |
| (1,1631) | 1:109:A:ARG:HB2 | 1:110:A:GLY:H | 2 | 0.2 | 0.06 | 0.2 |
| (1,1631) | 1:109:A:ARG:HB3 | 1:110:A:GLY:H | 2 | 0.2 | 0.06 | 0.2 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE1 | 2 | 0.2 | 0.01 | 0.2 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE2 | 2 | 0.2 | 0.01 | 0.2 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE3 | 2 | 0.2 | 0.01 | 0.2 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD11 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD12 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD13 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD11 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD12 | 2 | 0.2 | 0.06 | 0.2 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD13 | 2 | 0.2 | 0.06 | 0.2 |
| (1,709) | 1:11:A:THR:HG21 | 1:12:A:LEU:H | 2 | 0.2 | 0.02 | 0.2 |
| (1,709) | 1:11:A:THR:HG22 | 1:12:A:LEU:H | 2 | 0.2 | 0.02 | 0.2 |
| (1,709) | 1:11:A:THR:HG23 | 1:12:A:LEU:H | 2 | 0.2 | 0.02 | 0.2 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE1 | 2 | 0.19 | 0.05 | 0.19 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE2 | 2 | 0.19 | 0.05 | 0.19 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE3 | 2 | 0.19 | 0.05 | 0.19 |
| (1,388) | 1:86:A:GLY:HA2 | 1:98:A:PHE:HD2 | 2 | 0.18 | 0.02 | 0.18 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB1 | 2 | 0.18 | 0.08 | 0.18 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB2 | 2 | 0.18 | 0.08 | 0.18 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB3 | 2 | 0.18 | 0.08 | 0.18 |
| (1,1425) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB2 | 2 | 0.18 | 0.02 | 0.18 |

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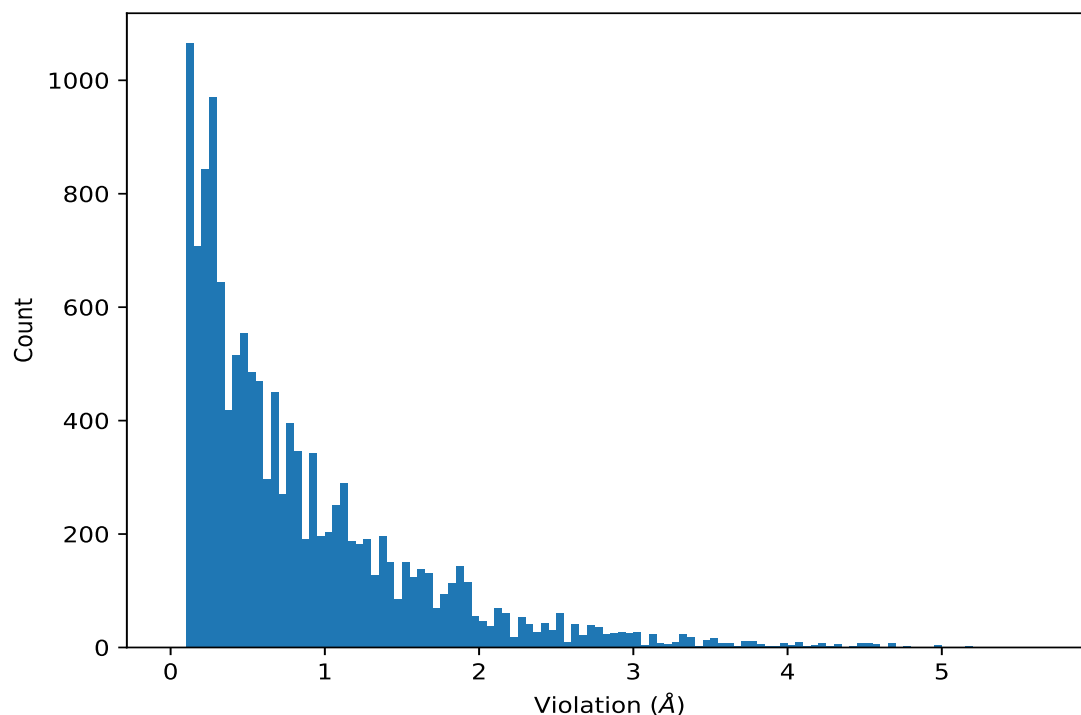
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1425) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,1605) | 1:98:A:PHE:HB2 | 1:100:A:ILE:H | 2 | 0.18 | 0.02 | 0.18 |
| (1,1605) | 1:98:A:PHE:HB3 | 1:100:A:ILE:H | 2 | 0.18 | 0.02 | 0.18 |
| (1,157) | 1:52:A:GLY:HA2 | 1:124:A:GLU:H | 2 | 0.18 | 0.04 | 0.18 |
| (1,624) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB3 | 2 | 0.18 | 0.02 | 0.18 |
| (1,808) | 1:43:A:GLY:H | 1:74:A:LEU:H | 2 | 0.17 | 0.0 | 0.17 |
| (1,799) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 2 | 0.16 | 0.04 | 0.16 |
| (1,1511) | 1:70:A:PHE:HB2 | 1:71:A:GLN:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,1511) | 1:70:A:PHE:HB3 | 1:71:A:GLN:H | 2 | 0.16 | 0.01 | 0.16 |
| (1,1009) | 1:76:A:ALA:H | 1:78:A:GLU:H | 2 | 0.16 | 0.05 | 0.16 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 2 | 0.16 | 0.02 | 0.16 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 2 | 0.16 | 0.02 | 0.16 |
| (1,680) | 1:50:A:TYR:HB3 | 1:50:A:TYR:HD1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,679) | 1:50:A:TYR:HB2 | 1:50:A:TYR:HD2 | 2 | 0.16 | 0.02 | 0.16 |
| (1,333) | 1:81:A:LYS:HA | 1:81:A:LYS:HD3 | 2 | 0.15 | 0.02 | 0.15 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG11 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG12 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG13 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG11 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG12 | 2 | 0.15 | 0.03 | 0.15 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG13 | 2 | 0.15 | 0.03 | 0.15 |
| (1,100) | 1:45:A:LYS:HB3 | 1:46:A:VAL:HA | 2 | 0.13 | 0.02 | 0.13 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG11 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG12 | 2 | 0.13 | 0.02 | 0.13 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG13 | 2 | 0.13 | 0.02 | 0.13 |
| (1,114) | 1:46:A:VAL:HG21 | 1:47:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,114) | 1:46:A:VAL:HG22 | 1:47:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,114) | 1:46:A:VAL:HG23 | 1:47:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,909) | 1:56:A:ASP:HA | 1:57:A:GLY:H | 2 | 0.12 | 0.01 | 0.12 |
| (1,748) | 1:27:A:GLU:H | 1:99:A:THR:HB | 2 | 0.12 | 0.0 | 0.12 |
| (1,45) | 1:34:A:GLY:HA3 | 1:94:A:GLU:HB2 | 2 | 0.11 | 0.0 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 20 | 5.69 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 9 | 5.47 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 8 | 5.4 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 7 | 5.38 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 20 | 5.31 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 20 | 5.23 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 14 | 5.18 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 7 | 5.16 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 5 | 5.15 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 8 | 5.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 4 | 4.98 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 12 | 4.97 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 8 | 4.96 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 2 | 4.95 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 13 | 4.91 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 12 | 4.78 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 5 | 4.75 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 5 | 4.68 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 5 | 4.68 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 5 | 4.68 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 5 | 4.68 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 5 | 4.68 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 5 | 4.68 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 3 | 4.66 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 17 | 4.6 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 9 | 4.58 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 9 | 4.58 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 9 | 4.58 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 6 | 4.56 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 13 | 4.55 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 3 | 4.54 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 2 | 4.51 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 2 | 4.51 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 2 | 4.51 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 2 | 4.51 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 2 | 4.51 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 2 | 4.51 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 18 | 4.49 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 12 | 4.48 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 19 | 4.47 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 19 | 4.47 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 19 | 4.47 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 4 | 4.46 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 4 | 4.46 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 4 | 4.46 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 2 | 4.44 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 2 | 4.44 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 8 | 4.43 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 3 | 4.33 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 5 | 4.31 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 5 | 4.31 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 14 | 4.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 14 | 4.31 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 15 | 4.3 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 6 | 4.27 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 19 | 4.25 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 16 | 4.24 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 3 | 4.22 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 3 | 4.22 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 15 | 4.22 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 13 | 4.22 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 18 | 4.21 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 5 | 4.21 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 10 | 4.2 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 9 | 4.19 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 8 | 4.17 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 3 | 4.15 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 3 | 4.15 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 3 | 4.15 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 17 | 4.14 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 12 | 4.11 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 9 | 4.11 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 3 | 4.1 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 15 | 4.1 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 19 | 4.09 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 12 | 4.07 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 15 | 4.06 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 15 | 4.06 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 15 | 4.06 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 15 | 4.06 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 15 | 4.06 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 9 | 4.02 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 6 | 4.01 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 20 | 4.01 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 5 | 4.0 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 13 | 3.99 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 14 | 3.98 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 10 | 3.98 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 10 | 3.98 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 10 | 3.98 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 3 | 3.96 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 15 | 3.95 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 6 | 3.95 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 10 | 3.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 2 | 3.91 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 9 | 3.91 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 3 | 3.9 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 17 | 3.89 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 16 | 3.88 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 12 | 3.83 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 12 | 3.83 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 18 | 3.83 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 20 | 3.83 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 14 | 3.81 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 16 | 3.81 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 4 | 3.79 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 7 | 3.79 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 7 | 3.79 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 7 | 3.79 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 15 | 3.78 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 15 | 3.78 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 15 | 3.78 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 20 | 3.77 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 17 | 3.77 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 3 | 3.76 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 7 | 3.75 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 4 | 3.74 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 5 | 3.73 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 8 | 3.73 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 17 | 3.73 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 10 | 3.71 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 10 | 3.71 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 10 | 3.71 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 10 | 3.71 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 10 | 3.71 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 10 | 3.71 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 9 | 3.7 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 18 | 3.68 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 7 | 3.66 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 20 | 3.64 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 20 | 3.64 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 10 | 3.64 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 10 | 3.63 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 19 | 3.62 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 19 | 3.62 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 19 | 3.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 4 | 3.58 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 4 | 3.58 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 4 | 3.58 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 6 | 3.57 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 17 | 3.57 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 10 | 3.56 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 15 | 3.56 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 2 | 3.55 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 6 | 3.55 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 6 | 3.55 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 6 | 3.55 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 4 | 3.54 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 8 | 3.53 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 8 | 3.53 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 6 | 3.52 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 6 | 3.52 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 12 | 3.52 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 1 | 3.51 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 18 | 3.51 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 8 | 3.5 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 19 | 3.5 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 19 | 3.5 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 19 | 3.5 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 5 | 3.49 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 14 | 3.49 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 15 | 3.48 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 9 | 3.48 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 4 | 3.47 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 4 | 3.47 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 4 | 3.47 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 18 | 3.46 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 3 | 3.46 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 16 | 3.46 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 16 | 3.46 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 16 | 3.46 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 7 | 3.46 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 4 | 3.43 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 1 | 3.43 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 3 | 3.41 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 3 | 3.4 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 3 | 3.4 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 1 | 3.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 5 | 3.4 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 5 | 3.4 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 5 | 3.4 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 4 | 3.4 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 4 | 3.4 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 4 | 3.4 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 17 | 3.39 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 3 | 3.39 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 14 | 3.38 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 1 | 3.38 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 17 | 3.37 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 17 | 3.37 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 14 | 3.36 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 14 | 3.36 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 14 | 3.36 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 8 | 3.36 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 2 | 3.34 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 2 | 3.34 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 2 | 3.34 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 13 | 3.33 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 13 | 3.33 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 9 | 3.33 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 9 | 3.33 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 1 | 3.33 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 4 | 3.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 4 | 3.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 4 | 3.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 4 | 3.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 4 | 3.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 4 | 3.32 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 19 | 3.32 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 19 | 3.32 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 4 | 3.32 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 4 | 3.32 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 4 | 3.32 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 7 | 3.32 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 7 | 3.32 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 7 | 3.32 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 14 | 3.31 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 7 | 3.3 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 8 | 3.3 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 5 | 3.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 7 | 3.26 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 7 | 3.26 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 12 | 3.26 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 17 | 3.26 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 17 | 3.26 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 17 | 3.26 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 19 | 3.25 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 4 | 3.23 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 15 | 3.22 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 15 | 3.22 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 15 | 3.22 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 3 | 3.21 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 16 | 3.2 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 9 | 3.19 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 1 | 3.18 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 1 | 3.18 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 1 | 3.18 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 4 | 3.18 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 2 | 3.17 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 14 | 3.17 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 11 | 3.16 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 18 | 3.15 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 5 | 3.14 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 5 | 3.14 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 2 | 3.14 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 5 | 3.14 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 5 | 3.14 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 5 | 3.14 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 4 | 3.13 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 20 | 3.13 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 9 | 3.12 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 9 | 3.12 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 9 | 3.12 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 17 | 3.11 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 17 | 3.11 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 17 | 3.11 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 10 | 3.1 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 10 | 3.1 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 9 | 3.1 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 11 | 3.1 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 11 | 3.1 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 11 | 3.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 4 | 3.1 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 4 | 3.1 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 4 | 3.1 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 2 | 3.09 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 15 | 3.07 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 15 | 3.07 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 15 | 3.07 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 6 | 3.07 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 18 | 3.05 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 18 | 3.05 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 18 | 3.05 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 12 | 3.05 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 17 | 3.04 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 16 | 3.04 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 16 | 3.04 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 16 | 3.04 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 9 | 3.03 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 20 | 3.03 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 13 | 3.02 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 13 | 3.02 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 13 | 3.02 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 19 | 3.02 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 1 | 3.02 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 1 | 3.02 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 1 | 3.02 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 19 | 3.01 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 19 | 3.01 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 2 | 3.01 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 9 | 3.0 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 3 | 3.0 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 3 | 3.0 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 3 | 3.0 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 6 | 3.0 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 6 | 3.0 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 6 | 3.0 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 10 | 2.99 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 14 | 2.99 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 3 | 2.99 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 3 | 2.99 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 3 | 2.99 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 4 | 2.99 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 10 | 2.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 10 | 2.98 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 16 | 2.97 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 16 | 2.97 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 13 | 2.97 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 12 | 2.97 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 12 | 2.97 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 12 | 2.97 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 15 | 2.97 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 9 | 2.96 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 9 | 2.96 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 9 | 2.96 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 9 | 2.96 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 9 | 2.96 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 19 | 2.96 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 6 | 2.95 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 16 | 2.95 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 20 | 2.95 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 5 | 2.95 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 11 | 2.95 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 20 | 2.94 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 2 | 2.94 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 16 | 2.94 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 1 | 2.94 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 10 | 2.94 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 10 | 2.94 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 10 | 2.94 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 4 | 2.94 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 6 | 2.94 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 10 | 2.93 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 16 | 2.93 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 16 | 2.93 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 16 | 2.93 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 17 | 2.93 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 17 | 2.93 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 17 | 2.93 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 12 | 2.93 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 1 | 2.92 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 19 | 2.92 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 19 | 2.92 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 19 | 2.92 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 14 | 2.92 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 15 | 2.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 15 | 2.91 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 15 | 2.91 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 15 | 2.91 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 15 | 2.91 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 15 | 2.91 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 5 | 2.9 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 20 | 2.89 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 20 | 2.89 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 5 | 2.89 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 13 | 2.89 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 17 | 2.88 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 17 | 2.88 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 17 | 2.88 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 17 | 2.88 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 17 | 2.88 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 17 | 2.88 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 16 | 2.88 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 16 | 2.88 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 16 | 2.88 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 16 | 2.88 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 16 | 2.88 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 16 | 2.88 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 20 | 2.88 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 8 | 2.87 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 8 | 2.87 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 11 | 2.87 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 4 | 2.87 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 4 | 2.87 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 4 | 2.87 |
| (1,530) | 1:106:A:TYR:HB3 | 1:111:A:TYR:HD2 | 8 | 2.85 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 18 | 2.84 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 18 | 2.84 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 8 | 2.84 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 8 | 2.84 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 8 | 2.84 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 17 | 2.84 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 17 | 2.84 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 9 | 2.83 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 11 | 2.83 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 7 | 2.83 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 7 | 2.83 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 7 | 2.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 8 | 2.82 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 7 | 2.81 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 2 | 2.81 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 4 | 2.81 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 8 | 2.81 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 8 | 2.81 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 8 | 2.81 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 7 | 2.81 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 7 | 2.81 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 7 | 2.81 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 4 | 2.81 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 8 | 2.8 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 8 | 2.8 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 12 | 2.8 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 12 | 2.8 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 12 | 2.8 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 18 | 2.79 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 18 | 2.79 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 3 | 2.79 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 20 | 2.79 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 7 | 2.79 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 4 | 2.78 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 4 | 2.78 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 4 | 2.78 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 4 | 2.78 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 4 | 2.78 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 4 | 2.78 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 2 | 2.78 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 16 | 2.78 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 8 | 2.78 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 8 | 2.78 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 8 | 2.78 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 4 | 2.78 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 2 | 2.77 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 10 | 2.76 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 2 | 2.75 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 2 | 2.75 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 11 | 2.75 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 15 | 2.75 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 15 | 2.75 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 15 | 2.75 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 16 | 2.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 16 | 2.75 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 16 | 2.75 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 16 | 2.75 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 16 | 2.75 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 16 | 2.75 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 15 | 2.74 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 16 | 2.74 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 20 | 2.73 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 8 | 2.73 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 8 | 2.73 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 8 | 2.73 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 12 | 2.73 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG11 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG12 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG13 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG21 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG22 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG23 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG11 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG12 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG13 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG21 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG22 | 3 | 2.72 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG23 | 3 | 2.72 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 7 | 2.72 |
| (1,530) | 1:106:A:TYR:HB3 | 1:111:A:TYR:HD2 | 7 | 2.72 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 3 | 2.72 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 3 | 2.72 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 3 | 2.72 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 20 | 2.71 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 20 | 2.71 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 20 | 2.71 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 20 | 2.71 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 20 | 2.71 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 9 | 2.71 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 2 | 2.71 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 8 | 2.71 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 9 | 2.7 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 9 | 2.7 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 8 | 2.7 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 8 | 2.7 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 8 | 2.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 17 | 2.7 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 10 | 2.7 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 20 | 2.69 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 1 | 2.69 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 3 | 2.69 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 7 | 2.68 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 7 | 2.68 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 7 | 2.68 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 17 | 2.68 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 17 | 2.68 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 17 | 2.68 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 13 | 2.67 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 13 | 2.67 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 13 | 2.67 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 13 | 2.67 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 13 | 2.67 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 13 | 2.67 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 17 | 2.67 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 17 | 2.66 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 7 | 2.66 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 7 | 2.66 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 7 | 2.66 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 10 | 2.66 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 15 | 2.66 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 13 | 2.65 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 7 | 2.65 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 11 | 2.65 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 10 | 2.65 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 7 | 2.64 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 7 | 2.64 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 7 | 2.64 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 4 | 2.63 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 4 | 2.63 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 7 | 2.63 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 1 | 2.63 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 1 | 2.63 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 1 | 2.63 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 15 | 2.63 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 15 | 2.63 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 15 | 2.63 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 15 | 2.62 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 15 | 2.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 15 | 2.62 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 15 | 2.62 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 15 | 2.62 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 15 | 2.62 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 3 | 2.62 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 7 | 2.62 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 20 | 2.62 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 19 | 2.62 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 17 | 2.62 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 6 | 2.61 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 6 | 2.61 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 6 | 2.61 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 6 | 2.61 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 6 | 2.61 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 6 | 2.61 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 3 | 2.61 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 8 | 2.6 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 8 | 2.6 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 1 | 2.6 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 1 | 2.6 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 1 | 2.6 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG21 | 20 | 2.6 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG22 | 20 | 2.6 |
| (1,480) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HG23 | 20 | 2.6 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 15 | 2.59 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 15 | 2.59 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 15 | 2.59 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 15 | 2.59 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 9 | 2.58 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 15 | 2.57 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 6 | 2.57 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 6 | 2.57 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 6 | 2.57 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 2 | 2.57 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 18 | 2.55 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 3 | 2.55 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 3 | 2.55 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 3 | 2.55 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 7 | 2.54 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 16 | 2.54 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 16 | 2.54 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 16 | 2.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 19 | 2.54 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 19 | 2.54 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 19 | 2.54 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 3 | 2.54 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 3 | 2.54 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 3 | 2.54 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 4 | 2.53 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 7 | 2.53 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 4 | 2.53 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 4 | 2.53 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 4 | 2.53 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 15 | 2.52 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 15 | 2.52 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 15 | 2.52 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 15 | 2.52 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 15 | 2.52 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 15 | 2.52 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 6 | 2.52 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 7 | 2.52 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 13 | 2.52 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 3 | 2.51 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 3 | 2.51 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 7 | 2.51 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 7 | 2.51 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 18 | 2.51 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 6 | 2.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,902) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 16 | 2.5 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 3 | 2.5 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 3 | 2.5 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 3 | 2.5 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 3 | 2.5 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 3 | 2.5 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 3 | 2.5 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 1 | 2.5 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 1 | 2.5 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 1 | 2.5 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 2 | 2.49 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 2 | 2.49 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 2 | 2.49 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 1 | 2.49 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 5 | 2.48 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 5 | 2.48 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 14 | 2.48 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 14 | 2.48 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 14 | 2.48 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 3 | 2.48 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 9 | 2.48 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 9 | 2.47 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 9 | 2.47 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 1 | 2.47 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 1 | 2.47 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 1 | 2.47 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 9 | 2.47 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 9 | 2.47 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 9 | 2.47 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 15 | 2.46 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 15 | 2.46 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 15 | 2.46 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 17 | 2.45 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 17 | 2.45 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 17 | 2.45 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 17 | 2.45 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 1 | 2.45 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 1 | 2.45 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 1 | 2.45 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 17 | 2.45 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 2 | 2.45 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 20 | 2.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 20 | 2.44 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 20 | 2.44 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 20 | 2.44 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 20 | 2.44 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 20 | 2.44 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 10 | 2.44 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 10 | 2.44 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 1 | 2.44 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 13 | 2.44 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 9 | 2.44 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 9 | 2.44 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 9 | 2.44 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 15 | 2.44 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 10 | 2.44 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 1 | 2.43 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 1 | 2.43 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 19 | 2.43 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 19 | 2.43 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 19 | 2.43 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 19 | 2.43 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 12 | 2.43 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 8 | 2.43 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 8 | 2.43 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 8 | 2.43 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 7 | 2.43 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 7 | 2.43 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 7 | 2.43 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 4 | 2.42 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 4 | 2.42 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 12 | 2.42 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 10 | 2.42 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 9 | 2.42 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 9 | 2.42 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 9 | 2.42 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 7 | 2.42 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 13 | 2.42 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 10 | 2.42 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 4 | 2.41 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 4 | 2.41 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 4 | 2.41 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 11 | 2.41 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 11 | 2.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 11 | 2.41 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 9 | 2.4 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 10 | 2.4 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 7 | 2.39 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 17 | 2.39 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 7 | 2.39 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 5 | 2.38 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 12 | 2.38 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 12 | 2.38 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 12 | 2.38 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 9 | 2.38 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 9 | 2.38 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 11 | 2.37 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 11 | 2.37 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 11 | 2.37 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 11 | 2.37 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 11 | 2.37 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 11 | 2.37 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 9 | 2.37 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 12 | 2.35 |
| (1,545) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 7 | 2.35 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 9 | 2.35 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 5 | 2.34 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 5 | 2.34 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 17 | 2.34 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 17 | 2.34 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 12 | 2.34 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 12 | 2.34 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 5 | 2.34 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 5 | 2.34 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 5 | 2.34 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 16 | 2.34 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 17 | 2.34 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 10 | 2.33 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 10 | 2.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 10 | 2.33 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 20 | 2.33 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 17 | 2.33 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 17 | 2.33 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 17 | 2.33 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 18 | 2.33 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 18 | 2.33 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 18 | 2.33 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 18 | 2.33 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 13 | 2.33 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 5 | 2.32 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 5 | 2.32 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 5 | 2.32 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 12 | 2.32 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 18 | 2.32 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 9 | 2.32 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 13 | 2.32 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 13 | 2.32 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 13 | 2.32 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 12 | 2.31 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 12 | 2.31 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 12 | 2.31 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 4 | 2.31 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 9 | 2.31 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 9 | 2.31 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 9 | 2.31 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 19 | 2.31 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 19 | 2.31 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 19 | 2.31 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 19 | 2.3 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 19 | 2.3 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 9 | 2.3 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 7 | 2.3 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 7 | 2.3 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 7 | 2.3 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 14 | 2.3 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 11 | 2.3 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 4 | 2.29 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 19 | 2.29 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 6 | 2.28 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 7 | 2.28 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 7 | 2.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 7 | 2.28 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 7 | 2.28 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 9 | 2.28 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 9 | 2.28 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 9 | 2.28 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 4 | 2.28 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 4 | 2.28 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 4 | 2.28 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 9 | 2.28 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 17 | 2.28 |
| (1,226) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 2 | 2.28 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 18 | 2.28 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 2 | 2.27 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 2 | 2.27 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 2 | 2.27 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 2 | 2.27 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 2 | 2.27 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 2 | 2.27 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 7 | 2.27 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 10 | 2.27 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 13 | 2.27 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 20 | 2.26 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 20 | 2.26 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 19 | 2.26 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 20 | 2.26 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 9 | 2.26 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 9 | 2.26 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 11 | 2.26 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 10 | 2.25 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 11 | 2.25 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 11 | 2.25 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 11 | 2.25 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 7 | 2.25 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 11 | 2.24 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 11 | 2.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 14 | 2.24 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 14 | 2.24 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 14 | 2.24 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 18 | 2.24 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 13 | 2.24 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 3 | 2.23 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 14 | 2.22 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 17 | 2.21 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 20 | 2.21 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 13 | 2.21 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 17 | 2.21 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 1 | 2.21 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 11 | 2.2 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 11 | 2.2 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 11 | 2.2 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 19 | 2.2 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 5 | 2.2 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 1 | 2.19 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 1 | 2.19 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 14 | 2.19 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 14 | 2.19 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 4 | 2.19 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 4 | 2.19 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 4 | 2.19 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 4 | 2.19 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 18 | 2.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 15 | 2.19 |
| (1,1600) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG2 | 9 | 2.18 |
| (1,1600) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG2 | 9 | 2.18 |
| (1,1600) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG2 | 9 | 2.18 |
| (1,1600) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG2 | 9 | 2.18 |
| (1,1600) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG2 | 9 | 2.18 |
| (1,1600) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG2 | 9 | 2.18 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 1 | 2.18 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 3 | 2.18 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 3 | 2.18 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 3 | 2.18 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 18 | 2.18 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 13 | 2.18 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 4 | 2.17 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 4 | 2.17 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 12 | 2.17 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 11 | 2.17 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 1 | 2.17 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 14 | 2.17 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 14 | 2.17 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 14 | 2.17 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 7 | 2.17 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 10 | 2.17 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 15 | 2.16 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 15 | 2.16 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 3 | 2.16 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 8 | 2.16 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 14 | 2.16 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 6 | 2.15 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 9 | 2.15 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 9 | 2.15 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 9 | 2.15 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 18 | 2.15 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 18 | 2.15 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 18 | 2.15 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 13 | 2.15 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 2 | 2.14 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 2 | 2.14 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 20 | 2.13 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 20 | 2.13 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 4 | 2.13 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 4 | 2.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 1 | 2.13 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 1 | 2.13 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 1 | 2.13 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 2 | 2.13 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 2 | 2.13 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 2 | 2.13 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 8 | 2.12 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 8 | 2.12 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 8 | 2.12 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 8 | 2.12 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 8 | 2.12 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 8 | 2.12 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 16 | 2.12 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 16 | 2.12 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 9 | 2.12 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 9 | 2.12 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 10 | 2.12 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 9 | 2.12 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 7 | 2.12 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 7 | 2.12 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 7 | 2.12 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 7 | 2.12 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 11 | 2.11 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 11 | 2.11 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 20 | 2.11 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 17 | 2.11 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 17 | 2.11 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 17 | 2.11 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 19 | 2.11 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 2 | 2.11 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 10 | 2.11 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 10 | 2.11 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 10 | 2.11 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 16 | 2.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 16 | 2.1 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 16 | 2.1 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 19 | 2.1 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 18 | 2.1 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 18 | 2.1 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 18 | 2.1 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 4 | 2.1 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 4 | 2.1 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 4 | 2.1 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 17 | 2.1 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 12 | 2.1 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 12 | 2.1 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 12 | 2.1 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 18 | 2.1 |
| (1,896) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 2 | 2.09 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 15 | 2.09 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 15 | 2.09 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 15 | 2.09 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 16 | 2.09 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 16 | 2.09 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 16 | 2.09 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 15 | 2.08 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 13 | 2.08 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 18 | 2.08 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 18 | 2.08 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 18 | 2.08 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 20 | 2.08 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 9 | 2.08 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 4 | 2.08 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 4 | 2.08 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 4 | 2.08 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 1 | 2.07 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 1 | 2.07 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 1 | 2.07 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 1 | 2.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 1 | 2.07 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 1 | 2.07 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 5 | 2.07 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 7 | 2.07 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 7 | 2.07 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 7 | 2.07 |
| (1,530) | 1:106:A:TYR:HB3 | 1:111:A:TYR:HD2 | 4 | 2.07 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 16 | 2.07 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 16 | 2.07 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 16 | 2.07 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 12 | 2.07 |
| (1,92) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 19 | 2.07 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 2 | 2.07 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 2 | 2.06 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 20 | 2.06 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 2 | 2.06 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 17 | 2.05 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 17 | 2.05 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 3 | 2.05 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 13 | 2.05 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 13 | 2.05 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 13 | 2.05 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 5 | 2.05 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 19 | 2.04 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 4 | 2.04 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 7 | 2.04 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 17 | 2.04 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 17 | 2.04 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 17 | 2.04 |
| (1,856) | 1:51:A:ASP:H | 1:123:A:PHE:HD2 | 10 | 2.03 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 7 | 2.03 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 7 | 2.03 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 7 | 2.03 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 13 | 2.03 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 13 | 2.03 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 13 | 2.03 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 16 | 2.03 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 9 | 2.02 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 9 | 2.02 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 17 | 2.02 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 16 | 2.02 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 16 | 2.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 16 | 2.02 |
| (1,395) | 1:40:A:PRO:HG2 | 1:88:A:ALA:HA | 7 | 2.02 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 3 | 2.02 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 3 | 2.02 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 3 | 2.02 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 16 | 2.02 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 15 | 2.01 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 14 | 2.01 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 7 | 2.01 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 7 | 2.01 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 7 | 2.01 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 13 | 2.0 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 16 | 2.0 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 16 | 2.0 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 16 | 2.0 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 19 | 2.0 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 19 | 2.0 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 19 | 2.0 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 13 | 2.0 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 7 | 2.0 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 5 | 2.0 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 3 | 1.99 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 3 | 1.99 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 3 | 1.99 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 3 | 1.99 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 3 | 1.99 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 3 | 1.99 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 4 | 1.99 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 4 | 1.99 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 4 | 1.99 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 4 | 1.98 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 15 | 1.98 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 10 | 1.98 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 3 | 1.98 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 1 | 1.98 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 1 | 1.98 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 1 | 1.98 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 1 | 1.98 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 19 | 1.98 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 13 | 1.98 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 1 | 1.98 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 8 | 1.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 2 | 1.98 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 2 | 1.98 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 2 | 1.98 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 16 | 1.97 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 16 | 1.97 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 16 | 1.97 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 16 | 1.97 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 16 | 1.97 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 16 | 1.97 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 8 | 1.97 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 3 | 1.97 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 3 | 1.97 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 15 | 1.97 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 5 | 1.97 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 5 | 1.97 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 5 | 1.97 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 9 | 1.97 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 9 | 1.97 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 9 | 1.97 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 5 | 1.97 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 17 | 1.96 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 17 | 1.96 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 17 | 1.96 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 17 | 1.96 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 17 | 1.96 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 17 | 1.96 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 7 | 1.96 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 7 | 1.96 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 7 | 1.96 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 3 | 1.96 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 4 | 1.96 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 4 | 1.96 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 4 | 1.96 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 3 | 1.96 |
| (1,1624) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 7 | 1.95 |
| (1,1624) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 7 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG2 | 8 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG2 | 8 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG2 | 8 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG2 | 8 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG2 | 8 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG2 | 8 | 1.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1600) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG2 | 19 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG2 | 19 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG2 | 19 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG2 | 19 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG2 | 19 | 1.95 |
| (1,1600) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG2 | 19 | 1.95 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 20 | 1.95 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 20 | 1.95 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 20 | 1.95 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 20 | 1.95 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 20 | 1.95 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 20 | 1.95 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 16 | 1.95 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 16 | 1.95 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 16 | 1.95 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 10 | 1.95 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 10 | 1.95 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 10 | 1.95 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 11 | 1.95 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 13 | 1.95 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 13 | 1.95 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 13 | 1.95 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 9 | 1.95 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 9 | 1.95 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 9 | 1.95 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 20 | 1.95 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 12 | 1.95 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 12 | 1.95 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 12 | 1.95 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 7 | 1.94 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 7 | 1.94 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 7 | 1.94 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 7 | 1.94 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 7 | 1.94 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 7 | 1.94 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 10 | 1.94 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 10 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 13 | 1.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 13 | 1.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 13 | 1.94 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 16 | 1.94 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 3 | 1.94 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 3 | 1.94 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 3 | 1.94 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 7 | 1.94 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 2 | 1.94 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 18 | 1.94 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 9 | 1.94 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 9 | 1.94 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 9 | 1.94 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 3 | 1.94 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 12 | 1.94 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 12 | 1.93 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 12 | 1.93 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 11 | 1.93 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 15 | 1.93 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 12 | 1.93 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 4 | 1.93 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 4 | 1.93 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 4 | 1.93 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 5 | 1.93 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 16 | 1.93 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 18 | 1.93 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 6 | 1.93 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 6 | 1.93 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 6 | 1.93 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 11 | 1.92 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 11 | 1.92 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 11 | 1.92 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 11 | 1.92 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 9 | 1.92 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 1 | 1.92 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 2 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 2 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 2 | 1.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 2 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 2 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 2 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 7 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 7 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 7 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 7 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 7 | 1.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 7 | 1.91 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 13 | 1.91 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 13 | 1.91 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 2 | 1.91 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 13 | 1.91 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 13 | 1.91 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 13 | 1.91 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 1 | 1.91 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 1 | 1.91 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 1 | 1.91 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 6 | 1.91 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 4 | 1.91 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 14 | 1.91 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 10 | 1.91 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 4 | 1.91 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 12 | 1.9 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 12 | 1.9 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 14 | 1.9 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 14 | 1.9 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 16 | 1.9 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 16 | 1.9 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 15 | 1.9 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 20 | 1.9 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 15 | 1.9 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 3 | 1.9 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 9 | 1.9 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 16 | 1.9 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 16 | 1.9 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 16 | 1.9 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 12 | 1.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 1 | 1.9 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 4 | 1.9 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 1 | 1.9 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 1 | 1.9 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 1 | 1.9 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 7 | 1.9 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 7 | 1.9 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 7 | 1.9 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 8 | 1.89 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 8 | 1.89 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 8 | 1.89 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 8 | 1.89 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 8 | 1.89 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 8 | 1.89 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 20 | 1.89 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 20 | 1.89 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 10 | 1.89 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 19 | 1.89 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 4 | 1.89 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 14 | 1.89 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 3 | 1.89 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 4 | 1.89 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 4 | 1.89 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 4 | 1.89 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 4 | 1.89 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 13 | 1.89 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 9 | 1.89 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 13 | 1.89 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 13 | 1.89 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 13 | 1.89 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 1 | 1.88 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 1 | 1.88 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 19 | 1.88 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 19 | 1.88 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 10 | 1.88 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 10 | 1.88 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 9 | 1.88 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 17 | 1.88 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 14 | 1.88 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 14 | 1.88 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 14 | 1.88 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 11 | 1.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 14 | 1.88 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 14 | 1.88 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 14 | 1.88 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 17 | 1.88 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 17 | 1.88 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 17 | 1.88 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 3 | 1.88 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 3 | 1.88 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 3 | 1.88 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 14 | 1.88 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG11 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG12 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG13 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG21 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG22 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG23 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG11 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG12 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG13 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG21 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG22 | 2 | 1.87 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG23 | 2 | 1.87 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 15 | 1.87 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 15 | 1.87 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 3 | 1.87 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 9 | 1.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 9 | 1.87 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 9 | 1.87 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 5 | 1.87 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 5 | 1.87 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 5 | 1.87 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 9 | 1.87 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 14 | 1.87 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 10 | 1.87 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 10 | 1.87 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 10 | 1.87 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 1 | 1.87 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 10 | 1.87 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 14 | 1.87 |
| (1,199) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 20 | 1.87 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 1 | 1.86 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 1 | 1.86 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 1 | 1.86 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 1 | 1.86 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 1 | 1.86 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 1 | 1.86 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 6 | 1.86 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 6 | 1.86 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 6 | 1.86 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 16 | 1.86 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 10 | 1.86 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 10 | 1.86 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 10 | 1.86 |
| (1,163) | 1:53:A:ARG:HG3 | 1:59:A:GLN:H | 12 | 1.86 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 2 | 1.86 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 15 | 1.86 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 20 | 1.86 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 20 | 1.86 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 20 | 1.86 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 9 | 1.85 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 13 | 1.85 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 9 | 1.85 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 13 | 1.85 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 18 | 1.85 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 19 | 1.85 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 6 | 1.85 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 3 | 1.84 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 3 | 1.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 3 | 1.84 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 3 | 1.84 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 3 | 1.84 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 3 | 1.84 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 17 | 1.84 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 17 | 1.84 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 17 | 1.84 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 7 | 1.84 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 8 | 1.84 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 8 | 1.84 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 8 | 1.84 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 8 | 1.84 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 8 | 1.84 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 8 | 1.84 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 5 | 1.84 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 7 | 1.84 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 7 | 1.84 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 7 | 1.84 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 18 | 1.84 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 12 | 1.83 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 12 | 1.83 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 2 | 1.83 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 2 | 1.83 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 2 | 1.83 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 3 | 1.83 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 11 | 1.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 11 | 1.83 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 11 | 1.83 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 20 | 1.83 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 17 | 1.82 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 17 | 1.82 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 17 | 1.82 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 17 | 1.82 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 17 | 1.82 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 17 | 1.82 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 13 | 1.82 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 13 | 1.82 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 10 | 1.82 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 10 | 1.82 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 16 | 1.82 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 16 | 1.82 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 16 | 1.82 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 10 | 1.82 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 13 | 1.82 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 1 | 1.82 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 5 | 1.82 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 13 | 1.81 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 13 | 1.81 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 13 | 1.81 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 13 | 1.81 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 13 | 1.81 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 13 | 1.81 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 16 | 1.81 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 16 | 1.81 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 16 | 1.81 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 16 | 1.81 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 16 | 1.81 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 16 | 1.81 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 15 | 1.81 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 15 | 1.81 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 15 | 1.81 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 15 | 1.81 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 15 | 1.81 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 15 | 1.81 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 1 | 1.81 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 15 | 1.81 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 15 | 1.81 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 15 | 1.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 9 | 1.81 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 2 | 1.81 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 2 | 1.81 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 2 | 1.81 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 4 | 1.81 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 10 | 1.81 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 10 | 1.81 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 10 | 1.81 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 2 | 1.81 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 2 | 1.81 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 2 | 1.81 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 12 | 1.81 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 4 | 1.8 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 4 | 1.8 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 4 | 1.8 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 4 | 1.8 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 4 | 1.8 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 4 | 1.8 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 16 | 1.8 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 16 | 1.8 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 16 | 1.8 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 4 | 1.8 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 13 | 1.8 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 13 | 1.8 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 13 | 1.8 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 8 | 1.8 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 8 | 1.8 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 8 | 1.8 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 19 | 1.79 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 19 | 1.79 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 19 | 1.79 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 19 | 1.79 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 10 | 1.79 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 19 | 1.79 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 19 | 1.79 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 19 | 1.79 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 6 | 1.79 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 6 | 1.79 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 6 | 1.79 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 6 | 1.79 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 18 | 1.78 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 18 | 1.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 7 | 1.78 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 16 | 1.78 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 20 | 1.78 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 7 | 1.77 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 7 | 1.77 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 7 | 1.77 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 7 | 1.77 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 7 | 1.77 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 7 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 3 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 3 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 3 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 3 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 3 | 1.77 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 3 | 1.77 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 1 | 1.77 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 1 | 1.77 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 1 | 1.77 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 1 | 1.77 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 1 | 1.77 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 1 | 1.77 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 8 | 1.77 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 8 | 1.77 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 17 | 1.77 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 1 | 1.77 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 1 | 1.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 1 | 1.77 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 7 | 1.77 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 7 | 1.77 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 7 | 1.77 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 15 | 1.77 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 15 | 1.77 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 15 | 1.77 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 16 | 1.77 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 7 | 1.77 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 14 | 1.77 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 4 | 1.77 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 4 | 1.77 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 4 | 1.77 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 4 | 1.77 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 3 | 1.76 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 18 | 1.76 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 6 | 1.76 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 15 | 1.76 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 15 | 1.76 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 15 | 1.76 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 9 | 1.76 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 4 | 1.76 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 1 | 1.76 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 13 | 1.76 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 13 | 1.76 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 13 | 1.76 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 14 | 1.76 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 14 | 1.76 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 14 | 1.76 |
| (1,1299) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 18 | 1.75 |
| (1,1299) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 18 | 1.75 |
| (1,1299) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 18 | 1.75 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 14 | 1.75 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 11 | 1.75 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 17 | 1.75 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 17 | 1.75 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 17 | 1.75 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 19 | 1.75 |
| (1,245) | 1:71:A:GLN:HA | 1:72:A:PHE:HD1 | 20 | 1.75 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 19 | 1.74 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 19 | 1.74 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 14 | 1.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 9 | 1.74 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 20 | 1.74 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 9 | 1.74 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 20 | 1.74 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 20 | 1.74 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 20 | 1.74 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 6 | 1.74 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 9 | 1.74 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 9 | 1.74 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 9 | 1.74 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 20 | 1.74 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 14 | 1.73 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 14 | 1.73 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 14 | 1.73 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 14 | 1.73 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 14 | 1.73 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 14 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG11 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG12 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG13 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG21 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG22 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG23 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG11 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG12 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG13 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG21 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG22 | 1 | 1.73 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG23 | 1 | 1.73 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 7 | 1.73 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 12 | 1.73 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 12 | 1.73 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 12 | 1.73 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 12 | 1.73 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 17 | 1.73 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 17 | 1.73 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 17 | 1.73 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 3 | 1.73 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 7 | 1.73 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 16 | 1.73 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 16 | 1.73 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 16 | 1.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 7 | 1.72 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 7 | 1.72 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 7 | 1.72 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 7 | 1.72 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 7 | 1.72 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 7 | 1.72 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 11 | 1.72 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 9 | 1.72 |
| (1,675) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB3 | 19 | 1.72 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 7 | 1.72 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 7 | 1.72 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 7 | 1.72 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 14 | 1.72 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 11 | 1.71 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 11 | 1.71 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 12 | 1.71 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 12 | 1.71 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 3 | 1.71 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 3 | 1.71 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 3 | 1.71 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 18 | 1.71 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 12 | 1.71 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 12 | 1.71 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 12 | 1.71 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 17 | 1.7 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 17 | 1.7 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 17 | 1.7 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 17 | 1.7 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 17 | 1.7 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 17 | 1.7 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 19 | 1.7 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 19 | 1.7 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 19 | 1.7 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 19 | 1.7 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 9 | 1.7 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 16 | 1.7 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 16 | 1.7 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 16 | 1.7 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 10 | 1.7 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 16 | 1.7 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 1 | 1.7 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 1 | 1.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 1 | 1.7 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 9 | 1.7 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 9 | 1.7 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 9 | 1.7 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 16 | 1.7 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 8 | 1.7 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 8 | 1.7 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 8 | 1.7 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 3 | 1.7 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 3 | 1.7 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 3 | 1.7 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 10 | 1.7 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 5 | 1.7 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 12 | 1.7 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 17 | 1.7 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 12 | 1.7 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 18 | 1.7 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 5 | 1.69 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 5 | 1.69 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 5 | 1.69 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 5 | 1.69 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 5 | 1.69 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 5 | 1.69 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG2 | 3 | 1.69 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG3 | 3 | 1.69 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 16 | 1.69 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 16 | 1.69 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 16 | 1.69 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 16 | 1.69 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 16 | 1.69 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 16 | 1.69 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 14 | 1.69 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 14 | 1.69 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 8 | 1.69 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 11 | 1.69 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 11 | 1.69 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 11 | 1.69 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 9 | 1.69 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 9 | 1.69 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 9 | 1.69 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 2 | 1.69 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 2 | 1.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 2 | 1.69 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 3 | 1.69 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 3 | 1.69 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 3 | 1.69 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 7 | 1.69 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 7 | 1.69 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 7 | 1.69 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 2 | 1.69 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 8 | 1.69 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 2 | 1.68 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 2 | 1.68 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 2 | 1.68 |
| (1,959) | 1:49:A:HIS:HD2 | 1:70:A:PHE:H | 4 | 1.68 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 19 | 1.68 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 12 | 1.68 |
| (1,205) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 8 | 1.68 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 20 | 1.68 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 10 | 1.68 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 10 | 1.68 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 10 | 1.68 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 13 | 1.68 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 13 | 1.68 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 13 | 1.68 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 4 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 4 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 4 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 4 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 4 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 4 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 7 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 7 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 7 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 7 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 7 | 1.67 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 7 | 1.67 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 5 | 1.67 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 10 | 1.67 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 10 | 1.67 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 10 | 1.67 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 9 | 1.67 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 9 | 1.67 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 9 | 1.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 20 | 1.67 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 20 | 1.67 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 20 | 1.67 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 13 | 1.67 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG11 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG12 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG13 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG21 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG22 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG23 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG11 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG12 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG13 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG21 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG22 | 5 | 1.66 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG23 | 5 | 1.66 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 11 | 1.66 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 11 | 1.66 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 11 | 1.66 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 7 | 1.66 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 6 | 1.66 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 6 | 1.66 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 6 | 1.66 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 18 | 1.66 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 13 | 1.66 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 1 | 1.66 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 4 | 1.66 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 4 | 1.66 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 4 | 1.66 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 7 | 1.66 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 11 | 1.65 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 20 | 1.65 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 4 | 1.65 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 4 | 1.65 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 4 | 1.65 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 16 | 1.65 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 1 | 1.65 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 1 | 1.65 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 1 | 1.65 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 1 | 1.65 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 1 | 1.65 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 1 | 1.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 6 | 1.65 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 11 | 1.65 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 11 | 1.65 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 11 | 1.65 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 3 | 1.64 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 3 | 1.64 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 3 | 1.64 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 3 | 1.64 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 3 | 1.64 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 3 | 1.64 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 4 | 1.64 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 4 | 1.64 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 4 | 1.64 |
| (1,706) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HB3 | 1 | 1.64 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 12 | 1.64 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 12 | 1.64 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 12 | 1.64 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 17 | 1.64 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 17 | 1.64 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 17 | 1.64 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 2 | 1.64 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 10 | 1.64 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 11 | 1.64 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 17 | 1.64 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 17 | 1.64 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 17 | 1.64 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 19 | 1.64 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 18 | 1.64 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 8 | 1.64 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 14 | 1.64 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 6 | 1.64 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 6 | 1.64 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 6 | 1.64 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 4 | 1.64 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 7 | 1.63 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 7 | 1.63 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 11 | 1.63 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 11 | 1.63 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 11 | 1.63 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 11 | 1.63 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG2 | 8 | 1.63 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG3 | 8 | 1.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG2 | 8 | 1.63 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG3 | 8 | 1.63 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG2 | 8 | 1.63 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG3 | 8 | 1.63 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 19 | 1.63 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 19 | 1.63 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 18 | 1.63 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 2 | 1.63 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 13 | 1.63 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 17 | 1.63 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 6 | 1.63 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 4 | 1.63 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 4 | 1.63 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 4 | 1.63 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 12 | 1.63 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 3 | 1.63 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 11 | 1.62 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 11 | 1.62 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 11 | 1.62 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 11 | 1.62 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 11 | 1.62 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 11 | 1.62 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 4 | 1.62 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 4 | 1.62 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 3 | 1.62 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 3 | 1.62 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 3 | 1.62 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 14 | 1.62 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 14 | 1.62 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 14 | 1.62 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 13 | 1.62 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 13 | 1.62 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 13 | 1.62 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 8 | 1.62 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 8 | 1.62 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 8 | 1.62 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 19 | 1.62 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 19 | 1.62 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 19 | 1.62 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 3 | 1.62 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 18 | 1.62 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 16 | 1.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 16 | 1.62 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 16 | 1.62 |
| (1,1475) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 20 | 1.61 |
| (1,1475) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 20 | 1.61 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 1 | 1.61 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 1 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG11 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG12 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG13 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG21 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG22 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG23 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG11 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG12 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG13 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG21 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG22 | 15 | 1.61 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG23 | 15 | 1.61 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 14 | 1.61 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 14 | 1.61 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 14 | 1.61 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 14 | 1.61 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 14 | 1.61 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 14 | 1.61 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 19 | 1.61 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 19 | 1.61 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 13 | 1.61 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 8 | 1.61 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 6 | 1.6 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 6 | 1.6 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 6 | 1.6 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 7 | 1.6 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 7 | 1.6 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 7 | 1.6 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 12 | 1.6 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 12 | 1.6 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 12 | 1.6 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 4 | 1.6 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 4 | 1.6 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 4 | 1.6 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 15 | 1.6 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 15 | 1.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 15 | 1.6 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 5 | 1.59 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 5 | 1.59 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 7 | 1.59 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 7 | 1.59 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 7 | 1.59 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 11 | 1.59 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 15 | 1.59 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 15 | 1.59 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 15 | 1.59 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 2 | 1.59 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 2 | 1.59 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 2 | 1.59 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 7 | 1.59 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 5 | 1.59 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 10 | 1.58 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 10 | 1.58 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 10 | 1.58 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 10 | 1.58 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 10 | 1.58 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 10 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 3 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 13 | 1.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 13 | 1.58 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 13 | 1.58 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 9 | 1.58 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 9 | 1.58 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 9 | 1.58 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 9 | 1.58 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 9 | 1.58 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 9 | 1.58 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 18 | 1.58 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 18 | 1.58 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 18 | 1.58 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 9 | 1.58 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 3 | 1.58 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 12 | 1.58 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 12 | 1.58 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 12 | 1.58 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 1 | 1.58 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 1 | 1.58 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 1 | 1.58 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 1 | 1.57 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 1 | 1.57 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 1 | 1.57 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 19 | 1.57 |
| (1,705) | 1:49:A:HIS:HE1 | 1:64:A:ARG:HA | 13 | 1.57 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 5 | 1.57 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 5 | 1.57 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 5 | 1.57 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 12 | 1.57 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 10 | 1.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 15 | 1.57 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 6 | 1.57 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 3 | 1.56 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 3 | 1.56 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 3 | 1.56 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 3 | 1.56 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 3 | 1.56 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 3 | 1.56 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 1 | 1.56 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 16 | 1.56 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 16 | 1.56 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 16 | 1.56 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 20 | 1.56 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 20 | 1.56 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 20 | 1.56 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 19 | 1.56 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 19 | 1.56 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 19 | 1.56 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 15 | 1.56 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 14 | 1.56 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 11 | 1.56 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 10 | 1.56 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 18 | 1.56 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 2 | 1.56 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 2 | 1.56 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 2 | 1.56 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 3 | 1.55 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 3 | 1.55 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 1 | 1.55 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 19 | 1.55 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 8 | 1.55 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 8 | 1.55 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 8 | 1.55 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 3 | 1.55 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 3 | 1.55 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 3 | 1.55 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 3 | 1.55 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 4 | 1.55 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 3 | 1.55 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 3 | 1.55 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 3 | 1.55 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 17 | 1.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 12 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 12 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 12 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 12 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 12 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 12 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 18 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 18 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 18 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 18 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 18 | 1.54 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 18 | 1.54 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 1 | 1.54 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 1 | 1.54 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 1 | 1.54 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 1 | 1.54 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 1 | 1.54 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 1 | 1.54 |
| (1,1173) | 1:102:A:TYR:H | 1:102:A:TYR:HE1 | 4 | 1.54 |
| (1,1173) | 1:102:A:TYR:H | 1:102:A:TYR:HE1 | 17 | 1.54 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 11 | 1.54 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 8 | 1.54 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 10 | 1.54 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 10 | 1.54 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 10 | 1.54 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 14 | 1.54 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 6 | 1.54 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 16 | 1.54 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 20 | 1.54 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 9 | 1.54 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 9 | 1.54 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 9 | 1.54 |
| (1,94) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG3 | 19 | 1.54 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 10 | 1.54 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 15 | 1.54 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 15 | 1.54 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 15 | 1.54 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 12 | 1.53 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 12 | 1.53 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 12 | 1.53 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 12 | 1.53 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 12 | 1.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 12 | 1.53 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 11 | 1.53 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 11 | 1.53 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 1 | 1.53 |
| (1,959) | 1:49:A:HIS:HD2 | 1:70:A:PHE:H | 16 | 1.53 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 20 | 1.53 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 16 | 1.53 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 16 | 1.53 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 8 | 1.53 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 13 | 1.53 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 13 | 1.53 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 17 | 1.53 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 15 | 1.52 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 15 | 1.52 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 15 | 1.52 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 15 | 1.52 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 15 | 1.52 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 15 | 1.52 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 1 | 1.52 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 1 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 19 | 1.52 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 19 | 1.52 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 12 | 1.52 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 2 | 1.52 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 20 | 1.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 20 | 1.52 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 20 | 1.52 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 13 | 1.52 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 13 | 1.52 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 13 | 1.52 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 4 | 1.52 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 1 | 1.52 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 1 | 1.52 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 1 | 1.52 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 12 | 1.52 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 12 | 1.52 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 12 | 1.52 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 4 | 1.52 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 4 | 1.52 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 4 | 1.52 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 3 | 1.52 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 6 | 1.52 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 6 | 1.52 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 6 | 1.52 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 6 | 1.52 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 8 | 1.52 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 8 | 1.52 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 8 | 1.52 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 16 | 1.52 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 16 | 1.52 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 16 | 1.52 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 2 | 1.52 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 2 | 1.52 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 2 | 1.52 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 4 | 1.52 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 11 | 1.52 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 11 | 1.51 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 11 | 1.51 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 11 | 1.51 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 11 | 1.51 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 11 | 1.51 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 11 | 1.51 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 13 | 1.51 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 13 | 1.51 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 20 | 1.51 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 20 | 1.51 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 14 | 1.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 14 | 1.51 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 14 | 1.51 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 14 | 1.51 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 2 | 1.51 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 2 | 1.51 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 2 | 1.51 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 15 | 1.51 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 15 | 1.51 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 15 | 1.51 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 16 | 1.51 |
| (1,462) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 14 | 1.51 |
| (1,462) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 14 | 1.51 |
| (1,462) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 14 | 1.51 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 4 | 1.51 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 10 | 1.51 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 11 | 1.51 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 11 | 1.51 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 11 | 1.51 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 3 | 1.51 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 8 | 1.5 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 4 | 1.5 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 12 | 1.5 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 8 | 1.5 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 11 | 1.5 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG2 | 18 | 1.49 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG3 | 18 | 1.49 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG2 | 18 | 1.49 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG3 | 18 | 1.49 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG2 | 18 | 1.49 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG3 | 18 | 1.49 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 17 | 1.49 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 17 | 1.49 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 3 | 1.49 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 1 | 1.49 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 15 | 1.49 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 15 | 1.49 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 15 | 1.49 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 8 | 1.49 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 7 | 1.49 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 1 | 1.49 |
| (1,395) | 1:40:A:PRO:HG2 | 1:88:A:ALA:HA | 11 | 1.49 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 3 | 1.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 11 | 1.48 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 11 | 1.48 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 10 | 1.48 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 15 | 1.48 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 17 | 1.48 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 16 | 1.48 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 1 | 1.48 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 1 | 1.47 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 1 | 1.47 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 18 | 1.47 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 19 | 1.47 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 19 | 1.47 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 19 | 1.47 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 9 | 1.47 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 9 | 1.47 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 9 | 1.47 |
| (1,528) | 1:80:A:ILE:HG21 | 1:106:A:TYR:HA | 9 | 1.47 |
| (1,528) | 1:80:A:ILE:HG22 | 1:106:A:TYR:HA | 9 | 1.47 |
| (1,528) | 1:80:A:ILE:HG23 | 1:106:A:TYR:HA | 9 | 1.47 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 16 | 1.47 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 16 | 1.47 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 16 | 1.47 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 16 | 1.47 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 16 | 1.47 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 16 | 1.47 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 16 | 1.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 16 | 1.47 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 16 | 1.47 |
| (1,522) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HA | 9 | 1.47 |
| (1,522) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HA | 9 | 1.47 |
| (1,522) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HA | 9 | 1.47 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 13 | 1.47 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 8 | 1.47 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 10 | 1.47 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 10 | 1.47 |
| (1,1655) | 1:126:A:GLU:HA | 1:128:A:LEU:HD11 | 9 | 1.46 |
| (1,1655) | 1:126:A:GLU:HA | 1:128:A:LEU:HD12 | 9 | 1.46 |
| (1,1655) | 1:126:A:GLU:HA | 1:128:A:LEU:HD13 | 9 | 1.46 |
| (1,1655) | 1:126:A:GLU:HA | 1:128:A:LEU:HD21 | 9 | 1.46 |
| (1,1655) | 1:126:A:GLU:HA | 1:128:A:LEU:HD22 | 9 | 1.46 |
| (1,1655) | 1:126:A:GLU:HA | 1:128:A:LEU:HD23 | 9 | 1.46 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 5 | 1.46 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 5 | 1.46 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 17 | 1.46 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 17 | 1.46 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 17 | 1.46 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 17 | 1.46 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 14 | 1.46 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 18 | 1.46 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 2 | 1.46 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 2 | 1.46 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 2 | 1.46 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 15 | 1.45 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 15 | 1.45 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 19 | 1.45 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 19 | 1.45 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 19 | 1.45 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 19 | 1.45 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 3 | 1.45 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 3 | 1.45 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 3 | 1.45 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 3 | 1.45 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 3 | 1.45 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 3 | 1.45 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 12 | 1.45 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 12 | 1.45 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 15 | 1.45 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 13 | 1.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 13 | 1.45 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 13 | 1.45 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 16 | 1.45 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 18 | 1.45 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 18 | 1.45 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 18 | 1.45 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 19 | 1.45 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 9 | 1.45 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 7 | 1.45 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 14 | 1.45 |
| (1,534) | 1:106:A:TYR:HB2 | 1:111:A:TYR:HD2 | 8 | 1.45 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 7 | 1.45 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 15 | 1.45 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 15 | 1.45 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 15 | 1.45 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 12 | 1.45 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 5 | 1.45 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 5 | 1.45 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 5 | 1.45 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 17 | 1.45 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 17 | 1.45 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 17 | 1.45 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 3 | 1.45 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 3 | 1.45 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 3 | 1.45 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 19 | 1.45 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 19 | 1.45 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 19 | 1.45 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 5 | 1.44 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 5 | 1.44 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 5 | 1.44 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 4 | 1.44 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 4 | 1.44 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 4 | 1.44 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 7 | 1.44 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 20 | 1.44 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 4 | 1.44 |
| (1,148) | 1:50:A:TYR:HB3 | 1:123:A:PHE:HD2 | 6 | 1.44 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 7 | 1.44 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 7 | 1.44 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 7 | 1.44 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 11 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 4 | 1.43 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 4 | 1.43 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 4 | 1.43 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 4 | 1.43 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 4 | 1.43 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 4 | 1.43 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 13 | 1.43 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 13 | 1.43 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 13 | 1.43 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 13 | 1.43 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 13 | 1.43 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 13 | 1.43 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB2 | 8 | 1.43 |
| (1,1479) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 8 | 1.43 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 12 | 1.43 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 8 | 1.43 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 12 | 1.43 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 18 | 1.43 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 3 | 1.43 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 15 | 1.43 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 4 | 1.43 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 17 | 1.43 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 17 | 1.43 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 17 | 1.43 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 6 | 1.43 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 6 | 1.43 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 6 | 1.43 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 14 | 1.43 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 14 | 1.43 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 14 | 1.43 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 19 | 1.43 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 19 | 1.43 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 19 | 1.43 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 6 | 1.43 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 9 | 1.43 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 13 | 1.43 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 5 | 1.43 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 15 | 1.43 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 4 | 1.42 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 4 | 1.42 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 4 | 1.42 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 4 | 1.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 4 | 1.42 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 4 | 1.42 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 1 | 1.42 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 17 | 1.42 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 13 | 1.42 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 13 | 1.42 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 13 | 1.42 |
| (1,226) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 10 | 1.42 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 12 | 1.42 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 9 | 1.41 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 9 | 1.41 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 6 | 1.41 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 6 | 1.41 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 6 | 1.41 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 6 | 1.41 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 6 | 1.41 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 6 | 1.41 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 16 | 1.41 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 16 | 1.41 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 16 | 1.41 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 16 | 1.41 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 8 | 1.41 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 8 | 1.41 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 8 | 1.41 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 8 | 1.41 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 8 | 1.41 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 8 | 1.41 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 5 | 1.41 |
| (1,1173) | 1:102:A:TYR:H | 1:102:A:TYR:HE1 | 18 | 1.41 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 13 | 1.41 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 13 | 1.41 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 13 | 1.41 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 16 | 1.41 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 10 | 1.41 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 10 | 1.41 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 10 | 1.41 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 20 | 1.41 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 6 | 1.41 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 8 | 1.41 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 8 | 1.41 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 8 | 1.41 |
| (1,444) | 1:31:A:LEU:HG | 1:95:A:LYS:HB3 | 1 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 5 | 1.41 |
| (1,206) | 1:60:A:PHE:HD1 | 1:61:A:ASP:HB3 | 8 | 1.41 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 11 | 1.41 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 11 | 1.41 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 11 | 1.41 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 9 | 1.41 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 9 | 1.41 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 9 | 1.41 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 19 | 1.4 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 19 | 1.4 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 19 | 1.4 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 19 | 1.4 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 19 | 1.4 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 19 | 1.4 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 11 | 1.4 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 11 | 1.4 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 11 | 1.4 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 11 | 1.4 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 11 | 1.4 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 11 | 1.4 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 1 | 1.4 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 1 | 1.4 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 1 | 1.4 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 5 | 1.4 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 5 | 1.4 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 5 | 1.4 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 20 | 1.4 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 20 | 1.4 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 20 | 1.4 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 3 | 1.4 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 3 | 1.4 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 3 | 1.4 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 16 | 1.4 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 16 | 1.4 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 16 | 1.4 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 4 | 1.4 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 8 | 1.4 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 17 | 1.4 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 17 | 1.4 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 17 | 1.4 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 6 | 1.4 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 1 | 1.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 13 | 1.4 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 19 | 1.4 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 13 | 1.39 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 13 | 1.39 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 15 | 1.39 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 15 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 7 | 1.39 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 7 | 1.39 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 14 | 1.39 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 14 | 1.39 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 16 | 1.39 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 16 | 1.39 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 1 | 1.39 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 1 | 1.39 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 1 | 1.39 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 15 | 1.39 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 15 | 1.39 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 15 | 1.39 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 17 | 1.39 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 17 | 1.39 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 17 | 1.39 |
| (1,1173) | 1:102:A:TYR:H | 1:102:A:TYR:HE1 | 7 | 1.39 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 6 | 1.39 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 14 | 1.39 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 15 | 1.39 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 2 | 1.39 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 2 | 1.39 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 2 | 1.39 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 3 | 1.39 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 3 | 1.39 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 3 | 1.39 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 2 | 1.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 2 | 1.39 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 2 | 1.39 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD11 | 9 | 1.39 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD12 | 9 | 1.39 |
| (1,567) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HD13 | 9 | 1.39 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 17 | 1.39 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 3 | 1.39 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 3 | 1.39 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 3 | 1.39 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 3 | 1.39 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 3 | 1.39 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 3 | 1.39 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 17 | 1.39 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 17 | 1.39 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 17 | 1.39 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 20 | 1.39 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 13 | 1.39 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 13 | 1.39 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 13 | 1.39 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 18 | 1.38 |
| (1,902) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 20 | 1.38 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 9 | 1.38 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 9 | 1.38 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 9 | 1.38 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 18 | 1.38 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 1 | 1.38 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 4 | 1.38 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 4 | 1.38 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 4 | 1.38 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 13 | 1.38 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 14 | 1.37 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 14 | 1.37 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 14 | 1.37 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 14 | 1.37 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 14 | 1.37 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 14 | 1.37 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 17 | 1.37 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 17 | 1.37 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 1 | 1.37 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 1 | 1.37 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 5 | 1.37 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 10 | 1.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 10 | 1.37 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 10 | 1.37 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 4 | 1.37 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 8 | 1.37 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 20 | 1.37 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 20 | 1.37 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 20 | 1.37 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB1 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB2 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB3 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB1 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB2 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB3 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB1 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB2 | 4 | 1.37 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB3 | 4 | 1.37 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 12 | 1.37 |
| (1,226) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 20 | 1.37 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 5 | 1.37 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 19 | 1.37 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 19 | 1.37 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 19 | 1.37 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 7 | 1.37 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 7 | 1.37 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 7 | 1.37 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 10 | 1.36 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 10 | 1.36 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 10 | 1.36 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 10 | 1.36 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 10 | 1.36 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 10 | 1.36 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 1 | 1.36 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 1 | 1.36 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 1 | 1.36 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 1 | 1.36 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 1 | 1.36 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 1 | 1.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 15 | 1.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 15 | 1.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 15 | 1.36 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 3 | 1.36 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 3 | 1.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 3 | 1.36 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 16 | 1.36 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 10 | 1.36 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 14 | 1.36 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD21 | 4 | 1.36 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD22 | 4 | 1.36 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD23 | 4 | 1.36 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 20 | 1.36 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 14 | 1.36 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 14 | 1.36 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 14 | 1.36 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 1 | 1.36 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 8 | 1.36 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 8 | 1.36 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 8 | 1.36 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 3 | 1.35 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 3 | 1.35 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 9 | 1.35 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 9 | 1.35 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 9 | 1.35 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 2 | 1.35 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 2 | 1.35 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 17 | 1.35 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 7 | 1.35 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 20 | 1.35 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 11 | 1.35 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 2 | 1.35 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 2 | 1.35 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 2 | 1.35 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 20 | 1.34 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 20 | 1.34 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 6 | 1.34 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 6 | 1.34 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 6 | 1.34 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 6 | 1.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 17 | 1.34 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 17 | 1.34 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 17 | 1.34 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 18 | 1.34 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 18 | 1.34 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 18 | 1.34 |
| (1,534) | 1:106:A:TYR:HB2 | 1:111:A:TYR:HD2 | 7 | 1.34 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 3 | 1.34 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 18 | 1.34 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 5 | 1.34 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 5 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 5 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 5 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 5 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 5 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 5 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 16 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 16 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 16 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 16 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 16 | 1.33 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 16 | 1.33 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 7 | 1.33 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 7 | 1.33 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 7 | 1.33 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 7 | 1.33 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 7 | 1.33 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 7 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 17 | 1.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 17 | 1.33 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 9 | 1.33 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 9 | 1.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 6 | 1.33 |
| (1,959) | 1:49:A:HIS:HD2 | 1:70:A:PHE:H | 10 | 1.33 |
| (1,609) | 1:123:A:PHE:HA | 1:124:A:GLU:HG3 | 9 | 1.33 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 7 | 1.33 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 7 | 1.33 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 7 | 1.33 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 13 | 1.33 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 13 | 1.33 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 13 | 1.33 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 8 | 1.33 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 1 | 1.33 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 1 | 1.33 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 1 | 1.33 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 15 | 1.33 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 15 | 1.33 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 15 | 1.33 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 15 | 1.32 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 18 | 1.32 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 19 | 1.32 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 11 | 1.32 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 12 | 1.32 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 12 | 1.32 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 12 | 1.32 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 6 | 1.31 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 6 | 1.31 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 6 | 1.31 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 6 | 1.31 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 6 | 1.31 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 6 | 1.31 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 16 | 1.31 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 16 | 1.31 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 3 | 1.31 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 7 | 1.31 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 7 | 1.31 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 7 | 1.31 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 12 | 1.31 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 19 | 1.31 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 17 | 1.31 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 18 | 1.31 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 18 | 1.31 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 18 | 1.31 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 8 | 1.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 8 | 1.31 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 8 | 1.31 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 5 | 1.31 |
| (1,558) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB2 | 4 | 1.31 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 5 | 1.31 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 5 | 1.31 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 5 | 1.31 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 13 | 1.31 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 13 | 1.31 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 13 | 1.31 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 1 | 1.31 |
| (1,279) | 1:75:A:GLY:HA3 | 1:84:A:ASP:HB3 | 11 | 1.31 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 19 | 1.31 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 8 | 1.31 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 8 | 1.31 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 8 | 1.31 |
| (1,1299) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 4 | 1.3 |
| (1,1299) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 4 | 1.3 |
| (1,1299) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 4 | 1.3 |
| (1,1299) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 10 | 1.3 |
| (1,1299) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 10 | 1.3 |
| (1,1299) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 10 | 1.3 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 4 | 1.3 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 15 | 1.3 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 8 | 1.3 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 8 | 1.3 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 8 | 1.3 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 17 | 1.3 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 17 | 1.3 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 17 | 1.3 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 18 | 1.3 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 4 | 1.3 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 7 | 1.3 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 7 | 1.3 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 7 | 1.3 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 17 | 1.3 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 1 | 1.3 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 16 | 1.29 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 12 | 1.29 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 12 | 1.29 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 12 | 1.29 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 7 | 1.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 14 | 1.29 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 14 | 1.29 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 14 | 1.29 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 11 | 1.29 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 11 | 1.29 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 11 | 1.29 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 6 | 1.29 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 6 | 1.29 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 6 | 1.29 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 6 | 1.29 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 6 | 1.29 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 6 | 1.29 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 1 | 1.29 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 1 | 1.29 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 1 | 1.29 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 15 | 1.29 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 19 | 1.29 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 1 | 1.28 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 1 | 1.28 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 1 | 1.28 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 1 | 1.28 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 1 | 1.28 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 1 | 1.28 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 17 | 1.28 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 6 | 1.28 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 6 | 1.28 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 6 | 1.28 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 18 | 1.28 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 18 | 1.28 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 18 | 1.28 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 16 | 1.28 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 16 | 1.28 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 16 | 1.28 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 14 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 3 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 3 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 3 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 16 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 16 | 1.28 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 16 | 1.28 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 3 | 1.28 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 13 | 1.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 4 | 1.28 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 4 | 1.28 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 4 | 1.28 |
| (1,371) | 1:81:A:LYS:HD3 | 1:84:A:ASP:HB2 | 14 | 1.28 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 12 | 1.28 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 2 | 1.28 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 18 | 1.28 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 18 | 1.28 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 18 | 1.28 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 13 | 1.28 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 13 | 1.28 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 13 | 1.28 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 9 | 1.28 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 9 | 1.28 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 9 | 1.28 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 13 | 1.27 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 13 | 1.27 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 2 | 1.27 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 2 | 1.27 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 2 | 1.27 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 2 | 1.27 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 2 | 1.27 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 2 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 12 | 1.27 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 12 | 1.27 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 1 | 1.27 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 1 | 1.27 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 1 | 1.27 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 7 | 1.27 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 3 | 1.27 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 1 | 1.27 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 17 | 1.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 11 | 1.27 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 11 | 1.27 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 11 | 1.27 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 7 | 1.27 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 7 | 1.27 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 7 | 1.27 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 13 | 1.27 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 13 | 1.27 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 13 | 1.27 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 17 | 1.27 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 17 | 1.27 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 17 | 1.27 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 13 | 1.27 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 13 | 1.27 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 13 | 1.27 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 6 | 1.27 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 20 | 1.27 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 20 | 1.27 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 20 | 1.27 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 3 | 1.27 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 4 | 1.27 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 13 | 1.26 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 13 | 1.26 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 13 | 1.26 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 13 | 1.26 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 13 | 1.26 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 13 | 1.26 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 4 | 1.26 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 4 | 1.26 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 16 | 1.26 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 16 | 1.26 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 6 | 1.26 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 6 | 1.26 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 6 | 1.26 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 6 | 1.26 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 6 | 1.26 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 6 | 1.26 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 13 | 1.26 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 13 | 1.26 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 13 | 1.26 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 13 | 1.26 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 13 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 13 | 1.26 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 1 | 1.26 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 12 | 1.26 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 8 | 1.26 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 8 | 1.26 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 8 | 1.26 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 18 | 1.26 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 18 | 1.26 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 18 | 1.26 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 6 | 1.26 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 16 | 1.26 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 16 | 1.26 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 16 | 1.26 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 3 | 1.26 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 13 | 1.26 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 17 | 1.26 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 10 | 1.26 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 10 | 1.26 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 10 | 1.26 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 16 | 1.26 |
| (1,417) | 1:90:A:MET:HE1 | 1:94:A:GLU:HG2 | 4 | 1.26 |
| (1,417) | 1:90:A:MET:HE2 | 1:94:A:GLU:HG2 | 4 | 1.26 |
| (1,417) | 1:90:A:MET:HE3 | 1:94:A:GLU:HG2 | 4 | 1.26 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 4 | 1.26 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 4 | 1.26 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 4 | 1.26 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 11 | 1.26 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 11 | 1.26 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 11 | 1.26 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 5 | 1.25 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 5 | 1.25 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 5 | 1.25 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 5 | 1.25 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 5 | 1.25 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 5 | 1.25 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 11 | 1.25 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 11 | 1.25 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 13 | 1.25 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 14 | 1.25 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 14 | 1.25 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 14 | 1.25 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 14 | 1.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 16 | 1.25 |
| (1,800) | 1:41:A:GLN:H | 1:44:A:LYS:HB2 | 6 | 1.25 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 2 | 1.25 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 2 | 1.25 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 2 | 1.25 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 10 | 1.25 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 10 | 1.25 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 10 | 1.25 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 11 | 1.25 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 15 | 1.25 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 13 | 1.25 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 13 | 1.25 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 13 | 1.25 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 1 | 1.25 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 1 | 1.25 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 1 | 1.25 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 3 | 1.25 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 3 | 1.25 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 3 | 1.25 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 18 | 1.24 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 18 | 1.24 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 18 | 1.24 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 18 | 1.24 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 18 | 1.24 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 18 | 1.24 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 15 | 1.24 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 15 | 1.24 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 15 | 1.24 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 5 | 1.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG21 | 15 | 1.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG22 | 15 | 1.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG23 | 15 | 1.24 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 13 | 1.24 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 13 | 1.24 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 13 | 1.24 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 20 | 1.24 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 20 | 1.24 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 20 | 1.24 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 6 | 1.24 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 6 | 1.24 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 6 | 1.24 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 17 | 1.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 17 | 1.24 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 17 | 1.24 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD21 | 13 | 1.24 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD22 | 13 | 1.24 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD23 | 13 | 1.24 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 19 | 1.24 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 18 | 1.24 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 18 | 1.24 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 18 | 1.24 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 14 | 1.24 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 3 | 1.24 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 3 | 1.24 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 3 | 1.24 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 12 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 12 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 12 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 12 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 12 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 12 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 15 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 15 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 15 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 15 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 15 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 15 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 20 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 20 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 20 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 20 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 20 | 1.23 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 20 | 1.23 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 9 | 1.23 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 9 | 1.23 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 9 | 1.23 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 9 | 1.23 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 9 | 1.23 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 9 | 1.23 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 7 | 1.23 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 7 | 1.23 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 7 | 1.23 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 7 | 1.23 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 7 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 7 | 1.23 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 16 | 1.23 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 16 | 1.23 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 16 | 1.23 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 16 | 1.23 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 16 | 1.23 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 16 | 1.23 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 20 | 1.23 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 20 | 1.23 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 17 | 1.23 |
| (1,903) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 16 | 1.23 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 16 | 1.23 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 6 | 1.23 |
| (1,674) | 1:106:A:TYR:HE1 | 1:111:A:TYR:HB2 | 19 | 1.23 |
| (1,673) | 1:52:A:GLY:HA3 | 1:123:A:PHE:HD1 | 2 | 1.23 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 4 | 1.23 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 4 | 1.23 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 4 | 1.23 |
| (1,560) | 1:106:A:TYR:HD1 | 1:111:A:TYR:HB3 | 19 | 1.23 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 19 | 1.23 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 19 | 1.23 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 19 | 1.23 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 2 | 1.23 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 9 | 1.23 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 9 | 1.23 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 9 | 1.23 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 3 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 3 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 3 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 3 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 3 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 3 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 18 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 18 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 18 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 18 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 18 | 1.22 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 18 | 1.22 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 16 | 1.22 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 16 | 1.22 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 16 | 1.22 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 16 | 1.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 18 | 1.22 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 12 | 1.22 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 8 | 1.22 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 16 | 1.22 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 1 | 1.22 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 1 | 1.22 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 1 | 1.22 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 13 | 1.22 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 19 | 1.22 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 19 | 1.22 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 19 | 1.22 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 14 | 1.22 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 14 | 1.22 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 14 | 1.22 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 2 | 1.22 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 2 | 1.22 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 2 | 1.22 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 17 | 1.22 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 17 | 1.22 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 17 | 1.22 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 14 | 1.22 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG21 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG22 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG23 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG21 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG22 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG23 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG21 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG22 | 9 | 1.22 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG23 | 9 | 1.22 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 3 | 1.22 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 9 | 1.22 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 10 | 1.22 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 10 | 1.22 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 10 | 1.22 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 19 | 1.21 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 19 | 1.21 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 19 | 1.21 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 19 | 1.21 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 19 | 1.21 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 19 | 1.21 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 19 | 1.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 19 | 1.21 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 19 | 1.21 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 19 | 1.21 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 19 | 1.21 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 19 | 1.21 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 8 | 1.21 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 8 | 1.21 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 8 | 1.21 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 8 | 1.21 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 8 | 1.21 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 8 | 1.21 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 7 | 1.21 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 7 | 1.21 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 7 | 1.21 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 7 | 1.21 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 7 | 1.21 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 7 | 1.21 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 15 | 1.21 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 9 | 1.21 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 17 | 1.21 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 8 | 1.21 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 6 | 1.21 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 6 | 1.21 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 6 | 1.21 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 11 | 1.21 |
| (1,594) | 1:122:A:VAL:HA | 1:123:A:PHE:HD1 | 9 | 1.21 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 10 | 1.21 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 20 | 1.21 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 19 | 1.21 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 11 | 1.21 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 13 | 1.21 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 13 | 1.21 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 13 | 1.21 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 5 | 1.2 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 5 | 1.2 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 5 | 1.2 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 5 | 1.2 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 5 | 1.2 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 5 | 1.2 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 12 | 1.2 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 12 | 1.2 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 12 | 1.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 12 | 1.2 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 12 | 1.2 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 12 | 1.2 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 19 | 1.2 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 17 | 1.2 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 3 | 1.2 |
| (1,772) | 1:32:A:THR:H | 1:95:A:LYS:HB3 | 1 | 1.2 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 2 | 1.2 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 2 | 1.2 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 2 | 1.2 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 4 | 1.2 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 4 | 1.2 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 4 | 1.2 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 2 | 1.2 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 2 | 1.2 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 2 | 1.2 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 12 | 1.2 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 16 | 1.2 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 8 | 1.2 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 8 | 1.2 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 8 | 1.2 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 4 | 1.2 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 4 | 1.2 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 4 | 1.2 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 4 | 1.2 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 4 | 1.2 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 4 | 1.2 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 18 | 1.2 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 18 | 1.2 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 18 | 1.2 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 16 | 1.2 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 16 | 1.2 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 16 | 1.2 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 19 | 1.2 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 4 | 1.2 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 1 | 1.19 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 1 | 1.19 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 1 | 1.19 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 1 | 1.19 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 1 | 1.19 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 1 | 1.19 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 13 | 1.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 13 | 1.19 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 11 | 1.19 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 11 | 1.19 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 2 | 1.19 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 14 | 1.19 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 11 | 1.19 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 15 | 1.19 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 13 | 1.19 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 13 | 1.19 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 13 | 1.19 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 15 | 1.19 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 17 | 1.19 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 18 | 1.19 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 18 | 1.19 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 18 | 1.19 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 20 | 1.19 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 13 | 1.19 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 15 | 1.19 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 15 | 1.19 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 15 | 1.19 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 5 | 1.19 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 5 | 1.19 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 5 | 1.19 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 6 | 1.19 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 5 | 1.19 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 5 | 1.19 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 18 | 1.19 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 16 | 1.19 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 16 | 1.19 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 16 | 1.19 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 15 | 1.19 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 3 | 1.19 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 5 | 1.19 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 10 | 1.19 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 1 | 1.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 1 | 1.18 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 1 | 1.18 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 1 | 1.18 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 10 | 1.18 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 10 | 1.18 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 19 | 1.18 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 19 | 1.18 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 16 | 1.18 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 16 | 1.18 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 16 | 1.18 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 14 | 1.18 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 16 | 1.18 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 10 | 1.18 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 9 | 1.18 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 15 | 1.18 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 15 | 1.18 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 15 | 1.18 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 9 | 1.18 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 9 | 1.18 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 9 | 1.18 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 5 | 1.18 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 5 | 1.18 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 5 | 1.18 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 13 | 1.18 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 13 | 1.18 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 13 | 1.18 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 6 | 1.18 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 19 | 1.17 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 19 | 1.17 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 17 | 1.17 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 17 | 1.17 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 17 | 1.17 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 17 | 1.17 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 2 | 1.17 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 2 | 1.17 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 2 | 1.17 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 2 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 14 | 1.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 14 | 1.17 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 14 | 1.17 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 3 | 1.17 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 3 | 1.17 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 3 | 1.17 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 5 | 1.17 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 1 | 1.17 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 3 | 1.17 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 4 | 1.17 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 17 | 1.17 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 2 | 1.17 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 4 | 1.17 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 6 | 1.17 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 6 | 1.17 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 6 | 1.17 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 10 | 1.17 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 5 | 1.17 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 1 | 1.16 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 1 | 1.16 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 4 | 1.16 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 4 | 1.16 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 8 | 1.16 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 7 | 1.16 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 20 | 1.16 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE1 | 2 | 1.16 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE2 | 2 | 1.16 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE3 | 2 | 1.16 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 19 | 1.16 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 19 | 1.16 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 19 | 1.16 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 3 | 1.16 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 3 | 1.16 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 3 | 1.16 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 4 | 1.16 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 4 | 1.16 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 4 | 1.16 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 17 | 1.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 5 | 1.16 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 5 | 1.16 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 5 | 1.16 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 3 | 1.16 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 12 | 1.16 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 12 | 1.16 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 12 | 1.16 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 11 | 1.16 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 19 | 1.16 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 1 | 1.16 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 2 | 1.16 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 6 | 1.15 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 7 | 1.15 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 13 | 1.15 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 13 | 1.15 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 13 | 1.15 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 3 | 1.15 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 3 | 1.15 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 3 | 1.15 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 1 | 1.15 |
| (1,681) | 1:50:A:TYR:H | 1:50:A:TYR:HD2 | 5 | 1.15 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 14 | 1.15 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 14 | 1.15 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 14 | 1.15 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 3 | 1.15 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 3 | 1.15 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 3 | 1.15 |
| (1,609) | 1:123:A:PHE:HA | 1:124:A:GLU:HG3 | 19 | 1.15 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD21 | 19 | 1.15 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD22 | 19 | 1.15 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD23 | 19 | 1.15 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 13 | 1.15 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 13 | 1.15 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 16 | 1.15 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 16 | 1.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 16 | 1.15 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 17 | 1.15 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 6 | 1.15 |
| (1,134) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HD1 | 12 | 1.15 |
| (1,134) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HD1 | 12 | 1.15 |
| (1,134) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HD1 | 12 | 1.15 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 19 | 1.15 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 19 | 1.15 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 19 | 1.15 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 8 | 1.15 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 8 | 1.15 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 8 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 1 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 1 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 1 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 7 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 7 | 1.15 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 7 | 1.15 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 10 | 1.14 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 10 | 1.14 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 10 | 1.14 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 10 | 1.14 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 10 | 1.14 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 10 | 1.14 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 2 | 1.14 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 2 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 9 | 1.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 9 | 1.14 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 9 | 1.14 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 3 | 1.14 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 19 | 1.14 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 19 | 1.14 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 19 | 1.14 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 10 | 1.14 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 1 | 1.14 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 1 | 1.14 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 1 | 1.14 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 15 | 1.14 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 5 | 1.14 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 5 | 1.14 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 5 | 1.14 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 18 | 1.14 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 5 | 1.14 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 7 | 1.14 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 17 | 1.14 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 17 | 1.14 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 17 | 1.14 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 12 | 1.14 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 7 | 1.14 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 4 | 1.14 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 4 | 1.14 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 4 | 1.14 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 9 | 1.14 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 9 | 1.14 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 9 | 1.14 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 13 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 13 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 13 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 13 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 13 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 13 | 1.13 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 19 | 1.13 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 19 | 1.13 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 5 | 1.13 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 20 | 1.13 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 20 | 1.13 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 20 | 1.13 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 2 | 1.13 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 18 | 1.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 18 | 1.13 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 18 | 1.13 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 2 | 1.13 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 2 | 1.13 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 2 | 1.13 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 4 | 1.13 |
| (1,609) | 1:123:A:PHE:HA | 1:124:A:GLU:HG3 | 8 | 1.13 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 5 | 1.13 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 19 | 1.13 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 18 | 1.13 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 5 | 1.13 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 5 | 1.13 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 19 | 1.13 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 16 | 1.13 |
| (1,195) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HA | 12 | 1.13 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 12 | 1.13 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 12 | 1.13 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 12 | 1.13 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 11 | 1.13 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 11 | 1.13 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 11 | 1.13 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 9 | 1.12 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 9 | 1.12 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 9 | 1.12 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 9 | 1.12 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 9 | 1.12 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 9 | 1.12 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 18 | 1.12 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 18 | 1.12 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 18 | 1.12 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 18 | 1.12 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 18 | 1.12 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 18 | 1.12 |
| (1,1299) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 14 | 1.12 |
| (1,1299) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 14 | 1.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1299) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 14 | 1.12 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 1 | 1.12 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 12 | 1.12 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 12 | 1.12 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 12 | 1.12 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 15 | 1.12 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 15 | 1.12 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 15 | 1.12 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 2 | 1.12 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 2 | 1.12 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 2 | 1.12 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 12 | 1.12 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 16 | 1.12 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 4 | 1.12 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 18 | 1.12 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 18 | 1.12 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 18 | 1.12 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 19 | 1.12 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 19 | 1.12 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 19 | 1.12 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 20 | 1.12 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 20 | 1.12 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 20 | 1.12 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 13 | 1.12 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 13 | 1.12 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 13 | 1.12 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD21 | 19 | 1.12 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD22 | 19 | 1.12 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD23 | 19 | 1.12 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 9 | 1.12 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 15 | 1.12 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 2 | 1.12 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 2 | 1.12 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 2 | 1.12 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 6 | 1.12 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 6 | 1.12 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 6 | 1.12 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 8 | 1.12 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 8 | 1.12 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 8 | 1.12 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 7 | 1.11 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 7 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 7 | 1.11 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 7 | 1.11 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 7 | 1.11 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 7 | 1.11 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 1 | 1.11 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 1 | 1.11 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 1 | 1.11 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 1 | 1.11 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 1 | 1.11 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 1 | 1.11 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 17 | 1.11 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 17 | 1.11 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 17 | 1.11 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 17 | 1.11 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 17 | 1.11 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 17 | 1.11 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG2 | 5 | 1.11 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG3 | 5 | 1.11 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG2 | 5 | 1.11 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG3 | 5 | 1.11 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG2 | 5 | 1.11 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG3 | 5 | 1.11 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 8 | 1.11 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 8 | 1.11 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 8 | 1.11 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 19 | 1.11 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 16 | 1.11 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 2 | 1.11 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 19 | 1.11 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 11 | 1.11 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 11 | 1.11 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 11 | 1.11 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 8 | 1.11 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 16 | 1.11 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 18 | 1.11 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 5 | 1.11 |
| (1,530) | 1:106:A:TYR:HB3 | 1:111:A:TYR:HD2 | 20 | 1.11 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 3 | 1.11 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 19 | 1.11 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 18 | 1.11 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 18 | 1.11 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 18 | 1.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 7 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 11 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 11 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 11 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 18 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 18 | 1.11 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 18 | 1.11 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 9 | 1.11 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 6 | 1.1 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 6 | 1.1 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 6 | 1.1 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 6 | 1.1 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 6 | 1.1 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 6 | 1.1 |
| (1,1253) | 1:123:A:PHE:HD2 | 1:124:A:GLU:H | 12 | 1.1 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 19 | 1.1 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 19 | 1.1 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 11 | 1.1 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 2 | 1.1 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 8 | 1.1 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 8 | 1.1 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 8 | 1.1 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 10 | 1.1 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 18 | 1.1 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 18 | 1.1 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 18 | 1.1 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 8 | 1.1 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 8 | 1.1 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 8 | 1.1 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 1 | 1.1 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 1 | 1.1 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 1 | 1.1 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 16 | 1.1 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 16 | 1.1 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 16 | 1.1 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 11 | 1.1 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 11 | 1.1 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 11 | 1.1 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 3 | 1.1 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 13 | 1.1 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG21 | 4 | 1.1 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG22 | 4 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG23 | 4 | 1.1 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 19 | 1.1 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 19 | 1.1 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 19 | 1.1 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 11 | 1.1 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 11 | 1.1 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 11 | 1.1 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 3 | 1.09 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 3 | 1.09 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 11 | 1.09 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 11 | 1.09 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 11 | 1.09 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 11 | 1.09 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 11 | 1.09 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 11 | 1.09 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 16 | 1.09 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 16 | 1.09 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 12 | 1.09 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 12 | 1.09 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 12 | 1.09 |
| (1,1130) | 1:90:A:MET:HE1 | 1:95:A:LYS:H | 4 | 1.09 |
| (1,1130) | 1:90:A:MET:HE2 | 1:95:A:LYS:H | 4 | 1.09 |
| (1,1130) | 1:90:A:MET:HE3 | 1:95:A:LYS:H | 4 | 1.09 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 12 | 1.09 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 12 | 1.09 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 12 | 1.09 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 1 | 1.09 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 1 | 1.09 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 1 | 1.09 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 2 | 1.09 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 7 | 1.09 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 5 | 1.09 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 4 | 1.09 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 3 | 1.09 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 8 | 1.09 |
| (1,545) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 13 | 1.09 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 11 | 1.09 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 11 | 1.09 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 11 | 1.09 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 15 | 1.09 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 15 | 1.09 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 15 | 1.09 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 8 | 1.09 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 8 | 1.09 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 8 | 1.09 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 12 | 1.09 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 12 | 1.09 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 12 | 1.09 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 18 | 1.09 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 18 | 1.09 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 18 | 1.09 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 19 | 1.09 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 10 | 1.09 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 15 | 1.09 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 1 | 1.09 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 8 | 1.09 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 20 | 1.09 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 20 | 1.09 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 20 | 1.09 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 3 | 1.08 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 3 | 1.08 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 3 | 1.08 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 3 | 1.08 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 3 | 1.08 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 3 | 1.08 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 11 | 1.08 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 11 | 1.08 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 11 | 1.08 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 11 | 1.08 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 11 | 1.08 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 11 | 1.08 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 5 | 1.08 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 5 | 1.08 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 5 | 1.08 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 16 | 1.08 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 12 | 1.08 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 8 | 1.08 |
| (1,903) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 2 | 1.08 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 11 | 1.08 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 11 | 1.08 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 11 | 1.08 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 20 | 1.08 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 9 | 1.08 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 6 | 1.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 6 | 1.08 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 6 | 1.08 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 15 | 1.08 |
| (1,587) | 1:115:A:ILE:HD11 | 1:121:A:LEU:HG | 4 | 1.08 |
| (1,587) | 1:115:A:ILE:HD12 | 1:121:A:LEU:HG | 4 | 1.08 |
| (1,587) | 1:115:A:ILE:HD13 | 1:121:A:LEU:HG | 4 | 1.08 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB1 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB2 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB3 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB1 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB2 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB3 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB1 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB2 | 11 | 1.08 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB3 | 11 | 1.08 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 5 | 1.08 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 16 | 1.08 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 20 | 1.08 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 15 | 1.07 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 15 | 1.07 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 7 | 1.07 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 7 | 1.07 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 7 | 1.07 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 7 | 1.07 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 7 | 1.07 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 7 | 1.07 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 8 | 1.07 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 8 | 1.07 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 14 | 1.07 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 14 | 1.07 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 14 | 1.07 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 14 | 1.07 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 14 | 1.07 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 14 | 1.07 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 10 | 1.07 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 10 | 1.07 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 10 | 1.07 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 4 | 1.07 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 11 | 1.07 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 3 | 1.07 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 9 | 1.07 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 17 | 1.07 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 18 | 1.07 |
| (1,677) | 1:105:A:ALA:HB1 | 1:106:A:TYR:HE2 | 18 | 1.07 |
| (1,677) | 1:105:A:ALA:HB2 | 1:106:A:TYR:HE2 | 18 | 1.07 |
| (1,677) | 1:105:A:ALA:HB3 | 1:106:A:TYR:HE2 | 18 | 1.07 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 10 | 1.07 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 10 | 1.07 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 10 | 1.07 |
| (1,450) | 1:32:A:THR:HB | 1:95:A:LYS:HE3 | 5 | 1.07 |
| (1,393) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HA | 4 | 1.07 |
| (1,393) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HA | 4 | 1.07 |
| (1,393) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HA | 4 | 1.07 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 17 | 1.07 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 17 | 1.07 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 17 | 1.07 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 12 | 1.07 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 7 | 1.07 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 8 | 1.06 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 8 | 1.06 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 8 | 1.06 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 8 | 1.06 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 8 | 1.06 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 8 | 1.06 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 14 | 1.06 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 14 | 1.06 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 9 | 1.06 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 18 | 1.06 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 15 | 1.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 10 | 1.06 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 19 | 1.06 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 7 | 1.06 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 7 | 1.06 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 7 | 1.06 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 6 | 1.06 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 6 | 1.06 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 6 | 1.06 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 18 | 1.06 |
| (1,39) | 1:32:A:THR:HB | 1:95:A:LYS:HB2 | 1 | 1.06 |
| (1,1658) | 1:126:A:GLU:HG3 | 1:128:A:LEU:HD11 | 9 | 1.05 |
| (1,1658) | 1:126:A:GLU:HG3 | 1:128:A:LEU:HD12 | 9 | 1.05 |
| (1,1658) | 1:126:A:GLU:HG3 | 1:128:A:LEU:HD13 | 9 | 1.05 |
| (1,1658) | 1:126:A:GLU:HG3 | 1:128:A:LEU:HD21 | 9 | 1.05 |
| (1,1658) | 1:126:A:GLU:HG3 | 1:128:A:LEU:HD22 | 9 | 1.05 |
| (1,1658) | 1:126:A:GLU:HG3 | 1:128:A:LEU:HD23 | 9 | 1.05 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 19 | 1.05 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 19 | 1.05 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 19 | 1.05 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 19 | 1.05 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 19 | 1.05 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 19 | 1.05 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 13 | 1.05 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 13 | 1.05 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 13 | 1.05 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 3 | 1.05 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 13 | 1.05 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 2 | 1.05 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 16 | 1.05 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 12 | 1.05 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 19 | 1.05 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 19 | 1.05 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 19 | 1.05 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 20 | 1.05 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 20 | 1.05 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 20 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 1 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 1 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 1 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 5 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 5 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 5 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 15 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 15 | 1.05 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 15 | 1.05 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 7 | 1.05 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 7 | 1.05 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 7 | 1.05 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 14 | 1.05 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 14 | 1.05 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 14 | 1.05 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 11 | 1.05 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 20 | 1.05 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 20 | 1.05 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 20 | 1.05 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 14 | 1.05 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 17 | 1.05 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 17 | 1.05 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 2 | 1.05 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 2 | 1.05 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 2 | 1.05 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 16 | 1.05 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 16 | 1.05 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 16 | 1.05 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 5 | 1.05 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 15 | 1.05 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 18 | 1.05 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 4 | 1.05 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 4 | 1.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 4 | 1.05 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 1 | 1.05 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 1 | 1.05 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 1 | 1.05 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 12 | 1.05 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 12 | 1.05 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 12 | 1.05 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 19 | 1.04 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 19 | 1.04 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 20 | 1.04 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 20 | 1.04 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 20 | 1.04 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 20 | 1.04 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 14 | 1.04 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 14 | 1.04 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 16 | 1.04 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 4 | 1.04 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 2 | 1.04 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 2 | 1.04 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 2 | 1.04 |
| (1,688) | 1:83:A:TRP:HD1 | 1:98:A:PHE:HD2 | 4 | 1.04 |
| (1,678) | 1:80:A:ILE:HD11 | 1:106:A:TYR:HE2 | 8 | 1.04 |
| (1,678) | 1:80:A:ILE:HD12 | 1:106:A:TYR:HE2 | 8 | 1.04 |
| (1,678) | 1:80:A:ILE:HD13 | 1:106:A:TYR:HE2 | 8 | 1.04 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 13 | 1.04 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 13 | 1.04 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 13 | 1.04 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 7 | 1.04 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 16 | 1.04 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 10 | 1.04 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 18 | 1.04 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 4 | 1.04 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 4 | 1.04 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 4 | 1.04 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 11 | 1.03 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 11 | 1.03 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 11 | 1.03 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 11 | 1.03 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 11 | 1.03 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 11 | 1.03 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 3 | 1.03 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 3 | 1.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 3 | 1.03 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 3 | 1.03 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 3 | 1.03 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 3 | 1.03 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 16 | 1.03 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 16 | 1.03 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 16 | 1.03 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 16 | 1.03 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 16 | 1.03 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 16 | 1.03 |
| (1,1262) | 1:123:A:PHE:HD2 | 1:125:A:VAL:H | 2 | 1.03 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 5 | 1.03 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 4 | 1.03 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 17 | 1.03 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 17 | 1.03 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 17 | 1.03 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 13 | 1.03 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 13 | 1.03 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 13 | 1.03 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 2 | 1.03 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 15 | 1.03 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 15 | 1.03 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 15 | 1.03 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 3 | 1.03 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 1 | 1.03 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 1 | 1.03 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 1 | 1.03 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 3 | 1.03 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 13 | 1.03 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 13 | 1.03 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 13 | 1.03 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 1 | 1.03 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 4 | 1.02 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 4 | 1.02 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 4 | 1.02 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 4 | 1.02 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 4 | 1.02 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 4 | 1.02 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 20 | 1.02 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 20 | 1.02 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 20 | 1.02 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 20 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 20 | 1.02 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 20 | 1.02 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 5 | 1.02 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 5 | 1.02 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 5 | 1.02 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 5 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 2 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 2 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 2 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 2 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 2 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 2 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 3 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 3 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 3 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 3 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 3 | 1.02 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 3 | 1.02 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 17 | 1.02 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 17 | 1.02 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 17 | 1.02 |
| (1,1064) | 1:81:A:LYS:HD3 | 1:85:A:GLN:H | 8 | 1.02 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 1 | 1.02 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 1 | 1.02 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 1 | 1.02 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 5 | 1.02 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 5 | 1.02 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 5 | 1.02 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 16 | 1.02 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 16 | 1.02 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 16 | 1.02 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 6 | 1.02 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 6 | 1.02 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 6 | 1.02 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 18 | 1.02 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 15 | 1.02 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 15 | 1.02 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 15 | 1.02 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 16 | 1.02 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD21 | 18 | 1.02 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD22 | 18 | 1.02 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD23 | 18 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 3 | 1.02 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 2 | 1.01 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 2 | 1.01 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 13 | 1.01 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 13 | 1.01 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 14 | 1.01 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 14 | 1.01 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 14 | 1.01 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 14 | 1.01 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 15 | 1.01 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 15 | 1.01 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 15 | 1.01 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 15 | 1.01 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 15 | 1.01 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 15 | 1.01 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 4 | 1.01 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 5 | 1.01 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 15 | 1.01 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 14 | 1.01 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 19 | 1.01 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 18 | 1.01 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 20 | 1.01 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 20 | 1.01 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 20 | 1.01 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 10 | 1.01 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 16 | 1.01 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 2 | 1.01 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 2 | 1.01 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 2 | 1.01 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 12 | 1.0 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 12 | 1.0 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 12 | 1.0 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 12 | 1.0 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 12 | 1.0 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 12 | 1.0 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 14 | 1.0 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 14 | 1.0 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 14 | 1.0 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 14 | 1.0 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 14 | 1.0 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 14 | 1.0 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 16 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 16 | 1.0 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 16 | 1.0 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 16 | 1.0 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 16 | 1.0 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 16 | 1.0 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 15 | 1.0 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 15 | 1.0 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 15 | 1.0 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 15 | 1.0 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 15 | 1.0 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 15 | 1.0 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 2 | 1.0 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 2 | 1.0 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 2 | 1.0 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 2 | 1.0 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 2 | 1.0 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 2 | 1.0 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 15 | 1.0 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 2 | 1.0 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 1 | 1.0 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 16 | 1.0 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 14 | 1.0 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 11 | 1.0 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 13 | 1.0 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 7 | 1.0 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 7 | 1.0 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 7 | 1.0 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 5 | 1.0 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 5 | 1.0 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 17 | 1.0 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 17 | 1.0 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 17 | 1.0 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 13 | 1.0 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 5 | 1.0 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 7 | 1.0 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 7 | 1.0 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 7 | 1.0 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG21 | 18 | 1.0 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG22 | 18 | 1.0 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG23 | 18 | 1.0 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 1 | 1.0 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 14 | 1.0 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 6 | 0.99 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 6 | 0.99 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 6 | 0.99 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 6 | 0.99 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 6 | 0.99 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 6 | 0.99 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 10 | 0.99 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 6 | 0.99 |
| (1,1199) | 1:80:A:ILE:HG21 | 1:105:A:ALA:H | 9 | 0.99 |
| (1,1199) | 1:80:A:ILE:HG22 | 1:105:A:ALA:H | 9 | 0.99 |
| (1,1199) | 1:80:A:ILE:HG23 | 1:105:A:ALA:H | 9 | 0.99 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 11 | 0.99 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 11 | 0.99 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 11 | 0.99 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 20 | 0.99 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 8 | 0.99 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 8 | 0.99 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 8 | 0.99 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE1 | 1 | 0.99 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE2 | 1 | 0.99 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE3 | 1 | 0.99 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 3 | 0.99 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 8 | 0.99 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 8 | 0.99 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 8 | 0.99 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 7 | 0.99 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 17 | 0.99 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 1 | 0.99 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 5 | 0.99 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 20 | 0.99 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 17 | 0.99 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 17 | 0.99 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 17 | 0.99 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 18 | 0.99 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 18 | 0.99 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 18 | 0.99 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 15 | 0.99 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 12 | 0.98 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 12 | 0.98 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 12 | 0.98 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 12 | 0.98 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 10 | 0.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 10 | 0.98 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 10 | 0.98 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 10 | 0.98 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 10 | 0.98 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 10 | 0.98 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 18 | 0.98 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 18 | 0.98 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE1 | 11 | 0.98 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE2 | 11 | 0.98 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE3 | 11 | 0.98 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 13 | 0.98 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 6 | 0.98 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 8 | 0.98 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 6 | 0.98 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 6 | 0.98 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 6 | 0.98 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 12 | 0.98 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 12 | 0.98 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 12 | 0.98 |
| (1,435) | 1:94:A:GLU:HA | 1:95:A:LYS:HB2 | 1 | 0.98 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 7 | 0.98 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 16 | 0.98 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 16 | 0.98 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 16 | 0.98 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 5 | 0.98 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 4 | 0.98 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 4 | 0.98 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 4 | 0.98 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 19 | 0.98 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 19 | 0.98 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 19 | 0.98 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 11 | 0.98 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 5 | 0.98 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 16 | 0.98 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 3 | 0.98 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 3 | 0.98 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 3 | 0.98 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 17 | 0.97 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 17 | 0.97 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 17 | 0.97 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 17 | 0.97 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 17 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 17 | 0.97 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 5 | 0.97 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 5 | 0.97 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 5 | 0.97 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 5 | 0.97 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 5 | 0.97 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 5 | 0.97 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 15 | 0.97 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 15 | 0.97 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 15 | 0.97 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 15 | 0.97 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 15 | 0.97 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 15 | 0.97 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 11 | 0.97 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 11 | 0.97 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 11 | 0.97 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 11 | 0.97 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 11 | 0.97 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 11 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 15 | 0.97 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 15 | 0.97 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 3 | 0.97 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 3 | 0.97 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 3 | 0.97 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 5 | 0.97 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 18 | 0.97 |
| (1,651) | 1:92:A:LEU:HD11 | 1:129:A:ALA:HA | 18 | 0.97 |
| (1,651) | 1:92:A:LEU:HD12 | 1:129:A:ALA:HA | 18 | 0.97 |
| (1,651) | 1:92:A:LEU:HD13 | 1:129:A:ALA:HA | 18 | 0.97 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 15 | 0.97 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 15 | 0.97 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 15 | 0.97 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 20 | 0.97 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 20 | 0.97 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 13 | 0.97 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 13 | 0.97 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 13 | 0.97 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 6 | 0.97 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 4 | 0.97 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 4 | 0.97 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 4 | 0.97 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 6 | 0.97 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 1 | 0.96 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 1 | 0.96 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 1 | 0.96 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 1 | 0.96 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 1 | 0.96 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 1 | 0.96 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 9 | 0.96 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 9 | 0.96 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 9 | 0.96 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 13 | 0.96 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 13 | 0.96 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 13 | 0.96 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 3 | 0.96 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 16 | 0.96 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 13 | 0.96 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 13 | 0.96 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 13 | 0.96 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB1 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB2 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB3 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB1 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB2 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB3 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB1 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB2 | 9 | 0.96 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB3 | 9 | 0.96 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 13 | 0.96 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 4 | 0.96 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 2 | 0.96 |
| (1,545) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 6 | 0.96 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 20 | 0.96 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 20 | 0.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 20 | 0.96 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 20 | 0.96 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 12 | 0.96 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 12 | 0.96 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 12 | 0.96 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 14 | 0.96 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 13 | 0.96 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 13 | 0.96 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 13 | 0.96 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 13 | 0.96 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 19 | 0.96 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 18 | 0.96 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 8 | 0.96 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 19 | 0.96 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 4 | 0.96 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 5 | 0.96 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG21 | 11 | 0.96 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG22 | 11 | 0.96 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG23 | 11 | 0.96 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 19 | 0.96 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 5 | 0.96 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 5 | 0.96 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 5 | 0.96 |
| (1,66) | 1:37:A:VAL:H | 1:38:A:THR:HG21 | 15 | 0.96 |
| (1,66) | 1:37:A:VAL:H | 1:38:A:THR:HG22 | 15 | 0.96 |
| (1,66) | 1:37:A:VAL:H | 1:38:A:THR:HG23 | 15 | 0.96 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 15 | 0.96 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 15 | 0.96 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 15 | 0.96 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 18 | 0.95 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 18 | 0.95 |
| (1,983) | 1:73:A:THR:H | 1:78:A:GLU:HB2 | 4 | 0.95 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 13 | 0.95 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 13 | 0.95 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 5 | 0.95 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 6 | 0.95 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 6 | 0.95 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 6 | 0.95 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 18 | 0.95 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 2 | 0.95 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 15 | 0.95 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 16 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 10 | 0.95 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 10 | 0.95 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 10 | 0.95 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 14 | 0.95 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 14 | 0.95 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 14 | 0.95 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 8 | 0.95 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 16 | 0.95 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 3 | 0.95 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 15 | 0.95 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 15 | 0.95 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 15 | 0.95 |
| (1,106) | 1:45:A:LYS:H | 1:45:A:LYS:HE3 | 16 | 0.95 |
| (1,93) | 1:41:A:GLN:HG3 | 1:44:A:LYS:HG2 | 19 | 0.95 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG21 | 11 | 0.95 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG22 | 11 | 0.95 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG23 | 11 | 0.95 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 13 | 0.95 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 3 | 0.95 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 3 | 0.95 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 3 | 0.95 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 4 | 0.94 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 4 | 0.94 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 20 | 0.94 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 20 | 0.94 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 1 | 0.94 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 1 | 0.94 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG2 | 4 | 0.94 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG3 | 4 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 8 | 0.94 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 8 | 0.94 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 13 | 0.94 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 6 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 10 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 10 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 10 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 13 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 13 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 13 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 17 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 17 | 0.94 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 17 | 0.94 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 8 | 0.94 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 6 | 0.94 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 6 | 0.94 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 6 | 0.94 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 5 | 0.94 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 5 | 0.94 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 5 | 0.94 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 2 | 0.94 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 2 | 0.94 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 2 | 0.94 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 13 | 0.94 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 13 | 0.94 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 13 | 0.94 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 1 | 0.94 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 11 | 0.94 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 11 | 0.94 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 11 | 0.94 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 8 | 0.94 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 8 | 0.94 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 8 | 0.94 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 12 | 0.94 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 12 | 0.94 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 12 | 0.94 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 14 | 0.94 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 14 | 0.94 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 14 | 0.94 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 10 | 0.94 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 10 | 0.94 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 10 | 0.94 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 4 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 4 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 4 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 4 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 4 | 0.93 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 4 | 0.93 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 15 | 0.93 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 15 | 0.93 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 15 | 0.93 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 15 | 0.93 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 15 | 0.93 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 15 | 0.93 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 12 | 0.93 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 12 | 0.93 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 8 | 0.93 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 8 | 0.93 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 8 | 0.93 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 8 | 0.93 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 7 | 0.93 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 7 | 0.93 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 7 | 0.93 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 7 | 0.93 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 7 | 0.93 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 7 | 0.93 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 5 | 0.93 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 5 | 0.93 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 5 | 0.93 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 5 | 0.93 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 5 | 0.93 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 5 | 0.93 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 4 | 0.93 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 17 | 0.93 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 11 | 0.93 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 11 | 0.93 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 11 | 0.93 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 6 | 0.93 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 15 | 0.93 |
| (1,1064) | 1:81:A:LYS:HD3 | 1:85:A:GLN:H | 19 | 0.93 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 16 | 0.93 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 16 | 0.93 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 16 | 0.93 |
| (1,1025) | 1:82:A:GLY:H | 1:104:A:LEU:HA | 1 | 0.93 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 18 | 0.93 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 18 | 0.93 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 18 | 0.93 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 1 | 0.93 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 1 | 0.93 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 1 | 0.93 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 19 | 0.93 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 14 | 0.93 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 14 | 0.93 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 14 | 0.93 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 7 | 0.93 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 2 | 0.93 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 1 | 0.93 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 1 | 0.93 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 1 | 0.93 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 12 | 0.93 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 12 | 0.93 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 12 | 0.93 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 20 | 0.93 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 20 | 0.93 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 20 | 0.93 |
| (1,449) | 1:32:A:THR:HB | 1:95:A:LYS:HE2 | 11 | 0.93 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 14 | 0.93 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 7 | 0.93 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 11 | 0.93 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 13 | 0.93 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 11 | 0.92 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 11 | 0.92 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 11 | 0.92 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 11 | 0.92 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 18 | 0.92 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 18 | 0.92 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 18 | 0.92 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 18 | 0.92 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 18 | 0.92 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 18 | 0.92 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 8 | 0.92 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 8 | 0.92 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 8 | 0.92 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 8 | 0.92 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 8 | 0.92 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 8 | 0.92 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 16 | 0.92 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 6 | 0.92 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 13 | 0.92 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 5 | 0.92 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 7 | 0.92 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 18 | 0.92 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 9 | 0.92 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 9 | 0.92 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 9 | 0.92 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 7 | 0.92 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 1 | 0.92 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 1 | 0.92 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 1 | 0.92 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 1 | 0.92 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 3 | 0.92 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 3 | 0.92 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 3 | 0.92 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 7 | 0.92 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 7 | 0.92 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 7 | 0.92 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 3 | 0.92 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 3 | 0.92 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 3 | 0.92 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 17 | 0.92 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 17 | 0.92 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 17 | 0.92 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 17 | 0.92 |
| (1,183) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 16 | 0.92 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 3 | 0.92 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 3 | 0.92 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 3 | 0.92 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 20 | 0.91 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 20 | 0.91 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 20 | 0.91 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 20 | 0.91 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 20 | 0.91 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 20 | 0.91 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 13 | 0.91 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 13 | 0.91 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 13 | 0.91 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 13 | 0.91 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 13 | 0.91 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 13 | 0.91 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 3 | 0.91 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 3 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 3 | 0.91 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 3 | 0.91 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 3 | 0.91 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 3 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 9 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 9 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 9 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 9 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 9 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 9 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 19 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 19 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 19 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 19 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 19 | 0.91 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 19 | 0.91 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 10 | 0.91 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 10 | 0.91 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 14 | 0.91 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 14 | 0.91 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 17 | 0.91 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 17 | 0.91 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 11 | 0.91 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 11 | 0.91 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 11 | 0.91 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 13 | 0.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 13 | 0.91 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 13 | 0.91 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 7 | 0.91 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 4 | 0.91 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 17 | 0.91 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 19 | 0.91 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 19 | 0.91 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 19 | 0.91 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 16 | 0.91 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 16 | 0.91 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 16 | 0.91 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 10 | 0.91 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 10 | 0.91 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 10 | 0.91 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 14 | 0.91 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 18 | 0.91 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 14 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 14 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 14 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 14 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 14 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 14 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 20 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 20 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 20 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 20 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 20 | 0.9 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 20 | 0.9 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 13 | 0.9 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 13 | 0.9 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 13 | 0.9 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 13 | 0.9 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 13 | 0.9 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 13 | 0.9 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 10 | 0.9 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 10 | 0.9 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 10 | 0.9 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 10 | 0.9 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 10 | 0.9 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 10 | 0.9 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 15 | 0.9 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 15 | 0.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 20 | 0.9 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 20 | 0.9 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 19 | 0.9 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 11 | 0.9 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 11 | 0.9 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 11 | 0.9 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 17 | 0.9 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 17 | 0.9 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 17 | 0.9 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 20 | 0.9 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 7 | 0.9 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 7 | 0.9 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 7 | 0.9 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 4 | 0.9 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 18 | 0.9 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 8 | 0.9 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 3 | 0.9 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 3 | 0.9 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 3 | 0.9 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 11 | 0.9 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 11 | 0.9 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 11 | 0.9 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD11 | 12 | 0.9 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD12 | 12 | 0.9 |
| (1,559) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HD13 | 12 | 0.9 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 3 | 0.9 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 3 | 0.9 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 3 | 0.9 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 4 | 0.9 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 8 | 0.9 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 10 | 0.9 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 10 | 0.9 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 10 | 0.9 |
| (1,167) | 1:53:A:ARG:HG2 | 1:54:A:PHE:HD1 | 4 | 0.9 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 9 | 0.9 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 20 | 0.89 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 20 | 0.89 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 20 | 0.89 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 20 | 0.89 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 20 | 0.89 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 20 | 0.89 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 19 | 0.89 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 19 | 0.89 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 3 | 0.89 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 3 | 0.89 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 7 | 0.89 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 7 | 0.89 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 11 | 0.89 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 12 | 0.89 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 2 | 0.89 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 2 | 0.89 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 2 | 0.89 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 2 | 0.89 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 4 | 0.89 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 4 | 0.89 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 4 | 0.89 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 14 | 0.89 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 14 | 0.89 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 14 | 0.89 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 19 | 0.89 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 9 | 0.89 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 11 | 0.89 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 7 | 0.89 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 7 | 0.89 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 7 | 0.89 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 7 | 0.89 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 1 | 0.89 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 18 | 0.89 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 18 | 0.89 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 18 | 0.89 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 1 | 0.89 |
| (1,449) | 1:32:A:THR:HB | 1:95:A:LYS:HE2 | 5 | 0.89 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 11 | 0.89 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 15 | 0.89 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 14 | 0.89 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 6 | 0.89 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 6 | 0.89 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 6 | 0.89 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 9 | 0.88 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 9 | 0.88 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 9 | 0.88 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 9 | 0.88 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 9 | 0.88 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 9 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 11 | 0.88 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 11 | 0.88 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 5 | 0.88 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 5 | 0.88 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE1 | 6 | 0.88 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE2 | 6 | 0.88 |
| (1,1085) | 1:89:A:THR:H | 1:90:A:MET:HE3 | 6 | 0.88 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 3 | 0.88 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 12 | 0.88 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 13 | 0.88 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 13 | 0.88 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 13 | 0.88 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 20 | 0.88 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 19 | 0.88 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 12 | 0.88 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 8 | 0.88 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 8 | 0.88 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 8 | 0.88 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 4 | 0.88 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 4 | 0.88 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 4 | 0.88 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 20 | 0.88 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 20 | 0.88 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 20 | 0.88 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 17 | 0.88 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 11 | 0.88 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 11 | 0.88 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 11 | 0.88 |
| (1,403) | 1:89:A:THR:HG21 | 1:98:A:PHE:HD2 | 1 | 0.88 |
| (1,403) | 1:89:A:THR:HG22 | 1:98:A:PHE:HD2 | 1 | 0.88 |
| (1,403) | 1:89:A:THR:HG23 | 1:98:A:PHE:HD2 | 1 | 0.88 |
| (1,393) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HA | 11 | 0.88 |
| (1,393) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HA | 11 | 0.88 |
| (1,393) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HA | 11 | 0.88 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 6 | 0.88 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 6 | 0.88 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 6 | 0.88 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 19 | 0.88 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 7 | 0.88 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 17 | 0.88 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 5 | 0.88 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 5 | 0.88 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 5 | 0.88 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 10 | 0.88 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 6 | 0.87 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 6 | 0.87 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 6 | 0.87 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 6 | 0.87 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 6 | 0.87 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 6 | 0.87 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 4 | 0.87 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 4 | 0.87 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 4 | 0.87 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 4 | 0.87 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 8 | 0.87 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 16 | 0.87 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 19 | 0.87 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 7 | 0.87 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 7 | 0.87 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 7 | 0.87 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 11 | 0.87 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 1 | 0.87 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 2 | 0.87 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 2 | 0.87 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 2 | 0.87 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 8 | 0.87 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 8 | 0.87 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 8 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,450) | 1:32:A:THR:HB | 1:95:A:LYS:HE3 | 11 | 0.87 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 13 | 0.87 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 13 | 0.87 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 13 | 0.87 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD21 | 1 | 0.87 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD22 | 1 | 0.87 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD23 | 1 | 0.87 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 6 | 0.87 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 6 | 0.87 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 6 | 0.87 |
| (1,192) | 1:59:A:GLN:HA | 1:61:A:ASP:H | 5 | 0.87 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 9 | 0.87 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 9 | 0.87 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 9 | 0.87 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 18 | 0.87 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 1 | 0.87 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 1 | 0.87 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 1 | 0.87 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 6 | 0.87 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 6 | 0.87 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 6 | 0.87 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 16 | 0.87 |
| (1,1475) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 16 | 0.86 |
| (1,1475) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 16 | 0.86 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 1 | 0.86 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 1 | 0.86 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 9 | 0.86 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 9 | 0.86 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 3 | 0.86 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 3 | 0.86 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 19 | 0.86 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 19 | 0.86 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 4 | 0.86 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 12 | 0.86 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 19 | 0.86 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 19 | 0.86 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 19 | 0.86 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 1 | 0.86 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 20 | 0.86 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 16 | 0.86 |
| (1,1025) | 1:82:A:GLY:H | 1:104:A:LEU:HA | 4 | 0.86 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 7 | 0.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 7 | 0.86 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 7 | 0.86 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 12 | 0.86 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 12 | 0.86 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 12 | 0.86 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 10 | 0.86 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 8 | 0.86 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 8 | 0.86 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 8 | 0.86 |
| (1,604) | 1:123:A:PHE:HD2 | 1:124:A:GLU:HA | 2 | 0.86 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 1 | 0.86 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 1 | 0.86 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 1 | 0.86 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 11 | 0.86 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 17 | 0.86 |
| (1,199) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 16 | 0.86 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 5 | 0.86 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 6 | 0.85 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 6 | 0.85 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 6 | 0.85 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 6 | 0.85 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 3 | 0.85 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 3 | 0.85 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 3 | 0.85 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 3 | 0.85 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 3 | 0.85 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 3 | 0.85 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 2 | 0.85 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 2 | 0.85 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 2 | 0.85 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 2 | 0.85 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 7 | 0.85 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 7 | 0.85 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 15 | 0.85 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 7 | 0.85 |
| (1,1105) | 1:38:A:THR:H | 1:92:A:LEU:H | 7 | 0.85 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 14 | 0.85 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 14 | 0.85 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 14 | 0.85 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 20 | 0.85 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 19 | 0.85 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 19 | 0.85 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 19 | 0.85 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 6 | 0.85 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 6 | 0.85 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 6 | 0.85 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 1 | 0.85 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 1 | 0.85 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 1 | 0.85 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 18 | 0.85 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 16 | 0.85 |
| (1,276) | 1:74:A:LEU:HD11 | 1:88:A:ALA:H | 4 | 0.85 |
| (1,276) | 1:74:A:LEU:HD12 | 1:88:A:ALA:H | 4 | 0.85 |
| (1,276) | 1:74:A:LEU:HD13 | 1:88:A:ALA:H | 4 | 0.85 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 15 | 0.85 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 15 | 0.85 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 15 | 0.85 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 4 | 0.85 |
| (1,226) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 15 | 0.85 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 5 | 0.85 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 10 | 0.85 |
| (1,92) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 3 | 0.85 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 1 | 0.85 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 1 | 0.85 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 1 | 0.85 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 6 | 0.85 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 6 | 0.85 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 6 | 0.85 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 3 | 0.84 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 3 | 0.84 |
| (1,1394) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HG2 | 3 | 0.84 |
| (1,1394) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HG3 | 3 | 0.84 |
| (1,1394) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HG2 | 3 | 0.84 |
| (1,1394) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HG3 | 3 | 0.84 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG11 | 3 | 0.84 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG12 | 3 | 0.84 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG13 | 3 | 0.84 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG21 | 3 | 0.84 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG22 | 3 | 0.84 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG23 | 3 | 0.84 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 17 | 0.84 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 17 | 0.84 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 4 | 0.84 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 20 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 19 | 0.84 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 1 | 0.84 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 1 | 0.84 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 1 | 0.84 |
| (1,800) | 1:41:A:GLN:H | 1:44:A:LYS:HB2 | 4 | 0.84 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 14 | 0.84 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 13 | 0.84 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 13 | 0.84 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 13 | 0.84 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 13 | 0.84 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 9 | 0.84 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 9 | 0.84 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 9 | 0.84 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 18 | 0.84 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 18 | 0.84 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 18 | 0.84 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 7 | 0.84 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 7 | 0.84 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 7 | 0.84 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 5 | 0.84 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 15 | 0.84 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 15 | 0.84 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 15 | 0.84 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 8 | 0.84 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 8 | 0.84 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 8 | 0.84 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 18 | 0.84 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 19 | 0.84 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 19 | 0.84 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 13 | 0.84 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 18 | 0.84 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 18 | 0.84 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 7 | 0.84 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 1 | 0.84 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 1 | 0.84 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 1 | 0.84 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 7 | 0.84 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 16 | 0.84 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 16 | 0.84 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 16 | 0.84 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 7 | 0.83 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 7 | 0.83 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 7 | 0.83 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 7 | 0.83 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 7 | 0.83 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 7 | 0.83 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 10 | 0.83 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 10 | 0.83 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 15 | 0.83 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 15 | 0.83 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 15 | 0.83 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 15 | 0.83 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 15 | 0.83 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 15 | 0.83 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 7 | 0.83 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 7 | 0.83 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 7 | 0.83 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 7 | 0.83 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 7 | 0.83 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 7 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG11 | 11 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG12 | 11 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG13 | 11 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG21 | 11 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG22 | 11 | 0.83 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG23 | 11 | 0.83 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 6 | 0.83 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 6 | 0.83 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 15 | 0.83 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 15 | 0.83 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 15 | 0.83 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 14 | 0.83 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 11 | 0.83 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 12 | 0.83 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 12 | 0.83 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 12 | 0.83 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 12 | 0.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 3 | 0.83 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 3 | 0.83 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 1 | 0.83 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 1 | 0.83 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 1 | 0.83 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 10 | 0.83 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 11 | 0.83 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 11 | 0.83 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 11 | 0.83 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 15 | 0.83 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 15 | 0.83 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 15 | 0.83 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 19 | 0.83 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 13 | 0.82 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 13 | 0.82 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 13 | 0.82 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 13 | 0.82 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 11 | 0.82 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 11 | 0.82 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 11 | 0.82 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 11 | 0.82 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 11 | 0.82 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 11 | 0.82 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 2 | 0.82 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 2 | 0.82 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 2 | 0.82 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 2 | 0.82 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 2 | 0.82 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 2 | 0.82 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 6 | 0.82 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 6 | 0.82 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 6 | 0.82 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 6 | 0.82 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 6 | 0.82 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 6 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 10 | 0.82 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 10 | 0.82 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 10 | 0.82 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 10 | 0.82 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 10 | 0.82 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 10 | 0.82 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 5 | 0.82 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 5 | 0.82 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 7 | 0.82 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 7 | 0.82 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 2 | 0.82 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 2 | 0.82 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 2 | 0.82 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 4 | 0.82 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 17 | 0.82 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 17 | 0.82 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 17 | 0.82 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 16 | 0.82 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 16 | 0.82 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 16 | 0.82 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 3 | 0.82 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 3 | 0.82 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 3 | 0.82 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 19 | 0.82 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 3 | 0.82 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 3 | 0.82 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 3 | 0.82 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 3 | 0.82 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 14 | 0.82 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 17 | 0.82 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 13 | 0.82 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 13 | 0.82 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 13 | 0.82 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 2 | 0.82 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 2 | 0.82 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 2 | 0.82 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 7 | 0.82 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 7 | 0.82 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 7 | 0.82 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 4 | 0.82 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 4 | 0.82 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 4 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 17 | 0.82 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 16 | 0.82 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 16 | 0.82 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 16 | 0.82 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 19 | 0.82 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 16 | 0.82 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 14 | 0.82 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 14 | 0.82 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 14 | 0.82 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 15 | 0.82 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 16 | 0.82 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 16 | 0.82 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 16 | 0.82 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 17 | 0.82 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 20 | 0.82 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 14 | 0.81 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 14 | 0.81 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 6 | 0.81 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 8 | 0.81 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 8 | 0.81 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 8 | 0.81 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 1 | 0.81 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 11 | 0.81 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 11 | 0.81 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 11 | 0.81 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 9 | 0.81 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 9 | 0.81 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 9 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 15 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 18 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 18 | 0.81 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 18 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 18 | 0.81 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 18 | 0.81 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 18 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 18 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 18 | 0.81 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 18 | 0.81 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 8 | 0.81 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 10 | 0.81 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 20 | 0.81 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 16 | 0.81 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 16 | 0.8 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 16 | 0.8 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 16 | 0.8 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 16 | 0.8 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 16 | 0.8 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 16 | 0.8 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 9 | 0.8 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 9 | 0.8 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 9 | 0.8 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 9 | 0.8 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 9 | 0.8 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 9 | 0.8 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 16 | 0.8 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 16 | 0.8 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 10 | 0.8 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 7 | 0.8 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 20 | 0.8 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 20 | 0.8 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 20 | 0.8 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 17 | 0.8 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 17 | 0.8 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 17 | 0.8 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 10 | 0.8 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 10 | 0.8 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 10 | 0.8 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 15 | 0.8 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 19 | 0.8 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 13 | 0.8 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 10 | 0.8 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 19 | 0.8 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 20 | 0.8 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 20 | 0.8 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 20 | 0.8 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 20 | 0.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 20 | 0.8 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 20 | 0.8 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 20 | 0.8 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 20 | 0.8 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 20 | 0.8 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 7 | 0.8 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 7 | 0.8 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 7 | 0.8 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG21 | 20 | 0.8 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG22 | 20 | 0.8 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG23 | 20 | 0.8 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 5 | 0.8 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 5 | 0.8 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 5 | 0.8 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 19 | 0.8 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 19 | 0.8 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 19 | 0.8 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 19 | 0.8 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 12 | 0.8 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 5 | 0.8 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 5 | 0.8 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 5 | 0.8 |
| (1,155) | 1:51:A:ASP:HB3 | 1:124:A:GLU:H | 20 | 0.8 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 20 | 0.8 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 8 | 0.8 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 8 | 0.8 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 8 | 0.8 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 14 | 0.8 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 3 | 0.79 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 3 | 0.79 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 18 | 0.79 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 18 | 0.79 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 18 | 0.79 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 18 | 0.79 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 18 | 0.79 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 18 | 0.79 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 9 | 0.79 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 9 | 0.79 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 9 | 0.79 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 9 | 0.79 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 9 | 0.79 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 9 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 6 | 0.79 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 6 | 0.79 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 10 | 0.79 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 10 | 0.79 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 8 | 0.79 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 1 | 0.79 |
| (1,1130) | 1:90:A:MET:HE1 | 1:95:A:LYS:H | 9 | 0.79 |
| (1,1130) | 1:90:A:MET:HE2 | 1:95:A:LYS:H | 9 | 0.79 |
| (1,1130) | 1:90:A:MET:HE3 | 1:95:A:LYS:H | 9 | 0.79 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 3 | 0.79 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 14 | 0.79 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 10 | 0.79 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 19 | 0.79 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 5 | 0.79 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 14 | 0.79 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 14 | 0.79 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 14 | 0.79 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 6 | 0.79 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 18 | 0.79 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 18 | 0.79 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 18 | 0.79 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 18 | 0.79 |
| (1,494) | 1:102:A:TYR:HB2 | 1:102:A:TYR:HE2 | 4 | 0.79 |
| (1,494) | 1:102:A:TYR:HB2 | 1:102:A:TYR:HE2 | 17 | 0.79 |
| (1,421) | 1:91:A:THR:HA | 1:127:A:LEU:HG | 7 | 0.79 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 16 | 0.79 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 15 | 0.79 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 15 | 0.79 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 15 | 0.79 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD21 | 1 | 0.79 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD22 | 1 | 0.79 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD23 | 1 | 0.79 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 19 | 0.79 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 19 | 0.79 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 19 | 0.79 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 15 | 0.79 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 15 | 0.79 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 17 | 0.79 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 17 | 0.79 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 17 | 0.79 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 17 | 0.79 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 18 | 0.79 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 18 | 0.79 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 18 | 0.79 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 5 | 0.79 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 5 | 0.79 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 5 | 0.79 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 15 | 0.79 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 16 | 0.78 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 16 | 0.78 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 16 | 0.78 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 16 | 0.78 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 16 | 0.78 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 16 | 0.78 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 15 | 0.78 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 15 | 0.78 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 7 | 0.78 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 7 | 0.78 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 7 | 0.78 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 7 | 0.78 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 1 | 0.78 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 1 | 0.78 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 1 | 0.78 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 1 | 0.78 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 1 | 0.78 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 1 | 0.78 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 13 | 0.78 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 13 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 13 | 0.78 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 9 | 0.78 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 17 | 0.78 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 17 | 0.78 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 17 | 0.78 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 17 | 0.78 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 2 | 0.78 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 16 | 0.78 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 18 | 0.78 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 18 | 0.78 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 18 | 0.78 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 19 | 0.78 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 19 | 0.78 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 19 | 0.78 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 8 | 0.78 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 8 | 0.78 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 8 | 0.78 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 13 | 0.78 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 20 | 0.78 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 20 | 0.78 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 20 | 0.78 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 19 | 0.78 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 2 | 0.78 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 8 | 0.78 |
| (1,689) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD1 | 4 | 0.78 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 8 | 0.78 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 12 | 0.78 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 12 | 0.78 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 12 | 0.78 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 15 | 0.78 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 15 | 0.78 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 15 | 0.78 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 15 | 0.78 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 8 | 0.78 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 5 | 0.78 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 5 | 0.78 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 5 | 0.78 |
| (1,494) | 1:102:A:TYR:HB2 | 1:102:A:TYR:HE2 | 18 | 0.78 |
| (1,394) | 1:74:A:LEU:HD11 | 1:88:A:ALA:HA | 4 | 0.78 |
| (1,394) | 1:74:A:LEU:HD12 | 1:88:A:ALA:HA | 4 | 0.78 |
| (1,394) | 1:74:A:LEU:HD13 | 1:88:A:ALA:HA | 4 | 0.78 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 11 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 19 | 0.78 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 19 | 0.78 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 19 | 0.78 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 5 | 0.78 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 5 | 0.78 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 5 | 0.78 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 18 | 0.78 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 18 | 0.78 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 18 | 0.78 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 14 | 0.78 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 5 | 0.78 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 6 | 0.78 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 16 | 0.78 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 2 | 0.78 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 14 | 0.78 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 14 | 0.78 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 14 | 0.78 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 9 | 0.78 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 9 | 0.78 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 9 | 0.78 |
| (1,92) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 12 | 0.78 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 11 | 0.78 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 11 | 0.78 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 11 | 0.78 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 18 | 0.78 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 13 | 0.77 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 13 | 0.77 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 13 | 0.77 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 13 | 0.77 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 13 | 0.77 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 13 | 0.77 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 13 | 0.77 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 13 | 0.77 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 2 | 0.77 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 2 | 0.77 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 2 | 0.77 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 2 | 0.77 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 2 | 0.77 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 2 | 0.77 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 1 | 0.77 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 1 | 0.77 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 1 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 1 | 0.77 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 1 | 0.77 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 1 | 0.77 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 6 | 0.77 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 6 | 0.77 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 3 | 0.77 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 2 | 0.77 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 2 | 0.77 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 2 | 0.77 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 6 | 0.77 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 6 | 0.77 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 6 | 0.77 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 4 | 0.77 |
| (1,802) | 1:41:A:GLN:H | 1:74:A:LEU:HB3 | 6 | 0.77 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 20 | 0.77 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 11 | 0.77 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 11 | 0.77 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 11 | 0.77 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 14 | 0.77 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 14 | 0.77 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 14 | 0.77 |
| (1,605) | 1:100:A:ILE:HD11 | 1:124:A:GLU:HA | 10 | 0.77 |
| (1,605) | 1:100:A:ILE:HD12 | 1:124:A:GLU:HA | 10 | 0.77 |
| (1,605) | 1:100:A:ILE:HD13 | 1:124:A:GLU:HA | 10 | 0.77 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 15 | 0.77 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 1 | 0.77 |
| (1,543) | 1:108:A:GLU:HA | 1:118:A:LYS:HG2 | 13 | 0.77 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 4 | 0.77 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 9 | 0.77 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 9 | 0.77 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 9 | 0.77 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 11 | 0.77 |
| (1,417) | 1:90:A:MET:HE1 | 1:94:A:GLU:HG2 | 9 | 0.77 |
| (1,417) | 1:90:A:MET:HE2 | 1:94:A:GLU:HG2 | 9 | 0.77 |
| (1,417) | 1:90:A:MET:HE3 | 1:94:A:GLU:HG2 | 9 | 0.77 |
| (1,403) | 1:89:A:THR:HG21 | 1:98:A:PHE:HD2 | 13 | 0.77 |
| (1,403) | 1:89:A:THR:HG22 | 1:98:A:PHE:HD2 | 13 | 0.77 |
| (1,403) | 1:89:A:THR:HG23 | 1:98:A:PHE:HD2 | 13 | 0.77 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 8 | 0.77 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 20 | 0.77 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 20 | 0.77 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 20 | 0.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 20 | 0.77 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 20 | 0.77 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 20 | 0.77 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 20 | 0.77 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 20 | 0.77 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 20 | 0.77 |
| (1,278) | 1:74:A:LEU:HD11 | 1:87:A:VAL:HB | 3 | 0.77 |
| (1,278) | 1:74:A:LEU:HD12 | 1:87:A:VAL:HB | 3 | 0.77 |
| (1,278) | 1:74:A:LEU:HD13 | 1:87:A:VAL:HB | 3 | 0.77 |
| (1,278) | 1:74:A:LEU:HD11 | 1:87:A:VAL:HB | 16 | 0.77 |
| (1,278) | 1:74:A:LEU:HD12 | 1:87:A:VAL:HB | 16 | 0.77 |
| (1,278) | 1:74:A:LEU:HD13 | 1:87:A:VAL:HB | 16 | 0.77 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 8 | 0.77 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 8 | 0.77 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 8 | 0.77 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 13 | 0.77 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 8 | 0.77 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 8 | 0.77 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 8 | 0.77 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 12 | 0.76 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 12 | 0.76 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 3 | 0.76 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 3 | 0.76 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 3 | 0.76 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 3 | 0.76 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 3 | 0.76 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 3 | 0.76 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 4 | 0.76 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 4 | 0.76 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 4 | 0.76 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 4 | 0.76 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 4 | 0.76 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 4 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 18 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 18 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 18 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 18 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 18 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 18 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 19 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 19 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 19 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 19 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 19 | 0.76 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 19 | 0.76 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 13 | 0.76 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 13 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 6 | 0.76 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 6 | 0.76 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 19 | 0.76 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 7 | 0.76 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 13 | 0.76 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 18 | 0.76 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 2 | 0.76 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 2 | 0.76 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 2 | 0.76 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 3 | 0.76 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 3 | 0.76 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 3 | 0.76 |
| (1,1096) | 1:91:A:THR:H | 1:94:A:GLU:H | 2 | 0.76 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 13 | 0.76 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 13 | 0.76 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 13 | 0.76 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 12 | 0.76 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 13 | 0.76 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 13 | 0.76 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 13 | 0.76 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 12 | 0.76 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 12 | 0.76 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 12 | 0.76 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 4 | 0.76 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 14 | 0.76 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 20 | 0.76 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 5 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 12 | 0.76 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 20 | 0.76 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 20 | 0.76 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 20 | 0.76 |
| (1,282) | 1:75:A:GLY:HA2 | 1:84:A:ASP:HB3 | 11 | 0.76 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 18 | 0.76 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 18 | 0.76 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 20 | 0.76 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 20 | 0.76 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 20 | 0.76 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 6 | 0.75 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 6 | 0.75 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 6 | 0.75 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 6 | 0.75 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 6 | 0.75 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 6 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 12 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 12 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 12 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 12 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 12 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 12 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 19 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 19 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 19 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 19 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 19 | 0.75 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 19 | 0.75 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 11 | 0.75 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 11 | 0.75 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 11 | 0.75 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 11 | 0.75 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 11 | 0.75 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 11 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 3 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 3 | 0.75 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 3 | 0.75 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 2 | 0.75 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 2 | 0.75 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 2 | 0.75 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 6 | 0.75 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 6 | 0.75 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 6 | 0.75 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 20 | 0.75 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 20 | 0.75 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 20 | 0.75 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 2 | 0.75 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 3 | 0.75 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 11 | 0.75 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 2 | 0.75 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 5 | 0.75 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 5 | 0.75 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 5 | 0.75 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 9 | 0.75 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 9 | 0.75 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 9 | 0.75 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 12 | 0.75 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 7 | 0.75 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 13 | 0.75 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 14 | 0.75 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 1 | 0.75 |
| (1,543) | 1:108:A:GLU:HA | 1:118:A:LYS:HG2 | 6 | 0.75 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 9 | 0.75 |
| (1,494) | 1:102:A:TYR:HB2 | 1:102:A:TYR:HE2 | 7 | 0.75 |
| (1,444) | 1:31:A:LEU:HG | 1:95:A:LYS:HB3 | 3 | 0.75 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 14 | 0.75 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 14 | 0.75 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 14 | 0.75 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 9 | 0.75 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 9 | 0.75 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 9 | 0.75 |
| (1,292) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HG2 | 15 | 0.75 |
| (1,292) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HG2 | 15 | 0.75 |
| (1,292) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HG2 | 15 | 0.75 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 4 | 0.75 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 2 | 0.75 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 2 | 0.75 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 2 | 0.75 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 16 | 0.75 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 6 | 0.74 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 6 | 0.74 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 8 | 0.74 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 8 | 0.74 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD2 | 13 | 0.74 |
| (1,1455) | 1:54:A:PHE:HD2 | 1:55:A:PRO:HD3 | 13 | 0.74 |
| (1,1393) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 19 | 0.74 |
| (1,1393) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG3 | 19 | 0.74 |
| (1,1393) | 1:41:A:GLN:HG3 | 1:44:A:LYS:HG2 | 19 | 0.74 |
| (1,1393) | 1:41:A:GLN:HG3 | 1:44:A:LYS:HG3 | 19 | 0.74 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 20 | 0.74 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 20 | 0.74 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 20 | 0.74 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 17 | 0.74 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 17 | 0.74 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 17 | 0.74 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 4 | 0.74 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 13 | 0.74 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 8 | 0.74 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 13 | 0.74 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 13 | 0.74 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 13 | 0.74 |
| (1,896) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 17 | 0.74 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 20 | 0.74 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 20 | 0.74 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 20 | 0.74 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 20 | 0.74 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 15 | 0.74 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 13 | 0.74 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 11 | 0.74 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 11 | 0.74 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 11 | 0.74 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 3 | 0.74 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 18 | 0.74 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 18 | 0.74 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 18 | 0.74 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 4 | 0.74 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 7 | 0.74 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 7 | 0.74 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 7 | 0.74 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 13 | 0.74 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 13 | 0.74 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 13 | 0.74 |
| (1,403) | 1:89:A:THR:HG21 | 1:98:A:PHE:HD2 | 2 | 0.74 |
| (1,403) | 1:89:A:THR:HG22 | 1:98:A:PHE:HD2 | 2 | 0.74 |
| (1,403) | 1:89:A:THR:HG23 | 1:98:A:PHE:HD2 | 2 | 0.74 |
| (1,403) | 1:89:A:THR:HG21 | 1:98:A:PHE:HD2 | 19 | 0.74 |
| (1,403) | 1:89:A:THR:HG22 | 1:98:A:PHE:HD2 | 19 | 0.74 |
| (1,403) | 1:89:A:THR:HG23 | 1:98:A:PHE:HD2 | 19 | 0.74 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 19 | 0.74 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 14 | 0.74 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 14 | 0.74 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 14 | 0.74 |
| (1,226) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 3 | 0.74 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 3 | 0.74 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 1 | 0.74 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 2 | 0.74 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 2 | 0.74 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 2 | 0.74 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 2 | 0.74 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 10 | 0.73 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 10 | 0.73 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 10 | 0.73 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 10 | 0.73 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 10 | 0.73 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 10 | 0.73 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 18 | 0.73 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 18 | 0.73 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 17 | 0.73 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 17 | 0.73 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 17 | 0.73 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 17 | 0.73 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 17 | 0.73 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 17 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 8 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 8 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 8 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 8 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 8 | 0.73 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 8 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 7 | 0.73 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 7 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 14 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 14 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 14 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 14 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 14 | 0.73 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 14 | 0.73 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 20 | 0.73 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 20 | 0.73 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 20 | 0.73 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 20 | 0.73 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 20 | 0.73 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 20 | 0.73 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 11 | 0.73 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 11 | 0.73 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 11 | 0.73 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 11 | 0.73 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 11 | 0.73 |
| (1,1374) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 11 | 0.73 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 11 | 0.73 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 11 | 0.73 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 5 | 0.73 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 5 | 0.73 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 5 | 0.73 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 14 | 0.73 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 8 | 0.73 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 8 | 0.73 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 8 | 0.73 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 7 | 0.73 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 7 | 0.73 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 7 | 0.73 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 20 | 0.73 |
| (1,910) | 1:55:A:PRO:HA | 1:57:A:GLY:H | 14 | 0.73 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 19 | 0.73 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 18 | 0.73 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 18 | 0.73 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 18 | 0.73 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 16 | 0.73 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 16 | 0.73 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 16 | 0.73 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 18 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 3 | 0.73 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 4 | 0.73 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 4 | 0.73 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 4 | 0.73 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 7 | 0.73 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 5 | 0.73 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 6 | 0.73 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 6 | 0.73 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 6 | 0.73 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 8 | 0.73 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 8 | 0.73 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 8 | 0.73 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 16 | 0.73 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 6 | 0.73 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 2 | 0.73 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 12 | 0.73 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 2 | 0.73 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 2 | 0.73 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 2 | 0.73 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 14 | 0.73 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 2 | 0.73 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 8 | 0.72 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 8 | 0.72 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 5 | 0.72 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 5 | 0.72 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 10 | 0.72 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 10 | 0.72 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 2 | 0.72 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 7 | 0.72 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 18 | 0.72 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 18 | 0.72 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 18 | 0.72 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 14 | 0.72 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 14 | 0.72 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 14 | 0.72 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 17 | 0.72 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 18 | 0.72 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 19 | 0.72 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 11 | 0.72 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 11 | 0.72 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 11 | 0.72 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 2 | 0.72 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 8 | 0.72 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 6 | 0.72 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 6 | 0.72 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 6 | 0.72 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 4 | 0.72 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 4 | 0.72 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 4 | 0.72 |
| (1,689) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD1 | 6 | 0.72 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 11 | 0.72 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 11 | 0.72 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 11 | 0.72 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 11 | 0.72 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 16 | 0.72 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 10 | 0.72 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 10 | 0.72 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 10 | 0.72 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 2 | 0.72 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 14 | 0.72 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 14 | 0.72 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 14 | 0.72 |
| (1,183) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 3 | 0.72 |
| (1,168) | 1:53:A:ARG:HG2 | 1:122:A:VAL:HB | 12 | 0.72 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 14 | 0.72 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 14 | 0.72 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 14 | 0.72 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 3 | 0.72 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 3 | 0.72 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 3 | 0.72 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 19 | 0.72 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 19 | 0.72 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 19 | 0.72 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 14 | 0.72 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 7 | 0.71 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 7 | 0.71 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 7 | 0.71 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 7 | 0.71 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 7 | 0.71 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 7 | 0.71 |
| (1,1575) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 7 | 0.71 |
| (1,1575) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 7 | 0.71 |
| (1,1575) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 7 | 0.71 |
| (1,1575) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 7 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1575) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 7 | 0.71 |
| (1,1575) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 7 | 0.71 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 12 | 0.71 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 12 | 0.71 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 17 | 0.71 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 17 | 0.71 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 10 | 0.71 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 9 | 0.71 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 9 | 0.71 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 9 | 0.71 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 6 | 0.71 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 3 | 0.71 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 5 | 0.71 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 4 | 0.71 |
| (1,762) | 1:31:A:LEU:H | 1:95:A:LYS:HB3 | 1 | 0.71 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 3 | 0.71 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 3 | 0.71 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 3 | 0.71 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 13 | 0.71 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 13 | 0.71 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 13 | 0.71 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 11 | 0.71 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 9 | 0.71 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 9 | 0.71 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 9 | 0.71 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 5 | 0.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 8 | 0.71 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 8 | 0.71 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 8 | 0.71 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 15 | 0.71 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 10 | 0.71 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 10 | 0.71 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 10 | 0.71 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD21 | 4 | 0.71 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD22 | 4 | 0.71 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD23 | 4 | 0.71 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 3 | 0.71 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 2 | 0.71 |
| (1,183) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 2 | 0.71 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 6 | 0.71 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 8 | 0.71 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 11 | 0.71 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 11 | 0.71 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 11 | 0.71 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 9 | 0.71 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 16 | 0.71 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 10 | 0.71 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 10 | 0.71 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 10 | 0.71 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 16 | 0.7 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 16 | 0.7 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 16 | 0.7 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 16 | 0.7 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 15 | 0.7 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 15 | 0.7 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 15 | 0.7 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 15 | 0.7 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 15 | 0.7 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 15 | 0.7 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 16 | 0.7 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 16 | 0.7 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 16 | 0.7 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 16 | 0.7 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 16 | 0.7 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 16 | 0.7 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 8 | 0.7 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 8 | 0.7 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 8 | 0.7 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 8 | 0.7 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 8 | 0.7 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 8 | 0.7 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 14 | 0.7 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 14 | 0.7 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 14 | 0.7 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 14 | 0.7 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 14 | 0.7 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 14 | 0.7 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 4 | 0.7 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 4 | 0.7 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 4 | 0.7 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 6 | 0.7 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 6 | 0.7 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 6 | 0.7 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 10 | 0.7 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 10 | 0.7 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 10 | 0.7 |
| (1,929) | 1:63:A:SER:H | 1:64:A:ARG:HG3 | 18 | 0.7 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 17 | 0.7 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 17 | 0.7 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 17 | 0.7 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 1 | 0.7 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 1 | 0.7 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 1 | 0.7 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 8 | 0.7 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 2 | 0.7 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 12 | 0.7 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 10 | 0.7 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 10 | 0.7 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 10 | 0.7 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 16 | 0.7 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 16 | 0.7 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 16 | 0.7 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 14 | 0.7 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 15 | 0.7 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 9 | 0.69 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 9 | 0.69 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 9 | 0.69 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 9 | 0.69 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 9 | 0.69 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 9 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 1 | 0.69 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 1 | 0.69 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 1 | 0.69 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 1 | 0.69 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 1 | 0.69 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 1 | 0.69 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 19 | 0.69 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 19 | 0.69 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 16 | 0.69 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 16 | 0.69 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 16 | 0.69 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 16 | 0.69 |
| (1,1299) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 15 | 0.69 |
| (1,1299) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 15 | 0.69 |
| (1,1299) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 15 | 0.69 |
| (1,1248) | 1:123:A:PHE:H | 1:123:A:PHE:HD1 | 14 | 0.69 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 6 | 0.69 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 6 | 0.69 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 6 | 0.69 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 10 | 0.69 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 10 | 0.69 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 10 | 0.69 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 1 | 0.69 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 19 | 0.69 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 17 | 0.69 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 17 | 0.69 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 17 | 0.69 |
| (1,959) | 1:49:A:HIS:HD2 | 1:70:A:PHE:H | 14 | 0.69 |
| (1,896) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 20 | 0.69 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 18 | 0.69 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 7 | 0.69 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 15 | 0.69 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 15 | 0.69 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 15 | 0.69 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 1 | 0.69 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 12 | 0.69 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 3 | 0.69 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 11 | 0.69 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 19 | 0.69 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 19 | 0.69 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 19 | 0.69 |
| (1,417) | 1:90:A:MET:HE1 | 1:94:A:GLU:HG2 | 7 | 0.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,417) | 1:90:A:MET:HE2 | 1:94:A:GLU:HG2 | 7 | 0.69 |
| (1,417) | 1:90:A:MET:HE3 | 1:94:A:GLU:HG2 | 7 | 0.69 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 3 | 0.69 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD21 | 13 | 0.69 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD22 | 13 | 0.69 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD23 | 13 | 0.69 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 9 | 0.69 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 9 | 0.69 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 9 | 0.69 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 1 | 0.69 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 14 | 0.69 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 14 | 0.69 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 14 | 0.69 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 1 | 0.69 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 4 | 0.69 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 14 | 0.69 |
| (1,1585) | 1:95:A:LYS:HG2 | 1:125:A:VAL:H | 1 | 0.68 |
| (1,1585) | 1:95:A:LYS:HG3 | 1:125:A:VAL:H | 1 | 0.68 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 13 | 0.68 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 13 | 0.68 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 13 | 0.68 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 13 | 0.68 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 13 | 0.68 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 13 | 0.68 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 6 | 0.68 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 6 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 20 | 0.68 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 20 | 0.68 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 4 | 0.68 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 4 | 0.68 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 4 | 0.68 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 13 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 13 | 0.68 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 13 | 0.68 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 13 | 0.68 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 20 | 0.68 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 20 | 0.68 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 20 | 0.68 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 7 | 0.68 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 1 | 0.68 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 1 | 0.68 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 1 | 0.68 |
| (1,929) | 1:63:A:SER:H | 1:64:A:ARG:HG3 | 14 | 0.68 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 1 | 0.68 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 12 | 0.68 |
| (1,689) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD1 | 14 | 0.68 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG21 | 7 | 0.68 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG22 | 7 | 0.68 |
| (1,669) | 1:111:A:TYR:HB3 | 1:115:A:ILE:HG23 | 7 | 0.68 |
| (1,651) | 1:92:A:LEU:HD11 | 1:129:A:ALA:HA | 14 | 0.68 |
| (1,651) | 1:92:A:LEU:HD12 | 1:129:A:ALA:HA | 14 | 0.68 |
| (1,651) | 1:92:A:LEU:HD13 | 1:129:A:ALA:HA | 14 | 0.68 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 3 | 0.68 |
| (1,545) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 3 | 0.68 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 5 | 0.68 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 5 | 0.68 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 5 | 0.68 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 14 | 0.68 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 14 | 0.68 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 14 | 0.68 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 18 | 0.68 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 8 | 0.68 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 8 | 0.68 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 3 | 0.68 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 20 | 0.68 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 20 | 0.68 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 20 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 20 | 0.68 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 20 | 0.68 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 20 | 0.68 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 8 | 0.68 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 2 | 0.68 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG21 | 12 | 0.68 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG22 | 12 | 0.68 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG23 | 12 | 0.68 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 3 | 0.68 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 6 | 0.68 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 6 | 0.68 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 6 | 0.68 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 4 | 0.68 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 9 | 0.68 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 8 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 8 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 8 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 8 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 8 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 8 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 19 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 19 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 19 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 19 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 19 | 0.67 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 19 | 0.67 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 14 | 0.67 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 14 | 0.67 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 14 | 0.67 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 14 | 0.67 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 14 | 0.67 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 14 | 0.67 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 11 | 0.67 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 11 | 0.67 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 11 | 0.67 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 11 | 0.67 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 11 | 0.67 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 11 | 0.67 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 16 | 0.67 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 16 | 0.67 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 16 | 0.67 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 16 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 16 | 0.67 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 16 | 0.67 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD11 | 12 | 0.67 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD12 | 12 | 0.67 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD13 | 12 | 0.67 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD21 | 12 | 0.67 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD22 | 12 | 0.67 |
| (1,1456) | 1:54:A:PHE:HD2 | 1:121:A:LEU:HD23 | 12 | 0.67 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 8 | 0.67 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 8 | 0.67 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 12 | 0.67 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 12 | 0.67 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 12 | 0.67 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 12 | 0.67 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG2 | 6 | 0.67 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG3 | 6 | 0.67 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 9 | 0.67 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 9 | 0.67 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 9 | 0.67 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 9 | 0.67 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 9 | 0.67 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 9 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 4 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 4 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 4 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 4 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 4 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 4 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 9 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 9 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 9 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 9 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 9 | 0.67 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 9 | 0.67 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 18 | 0.67 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 18 | 0.67 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 9 | 0.67 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 9 | 0.67 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 9 | 0.67 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 11 | 0.67 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 16 | 0.67 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 9 | 0.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 9 | 0.67 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 9 | 0.67 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 14 | 0.67 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 9 | 0.67 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 7 | 0.67 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 7 | 0.67 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 7 | 0.67 |
| (1,587) | 1:115:A:ILE:HD11 | 1:121:A:LEU:HG | 8 | 0.67 |
| (1,587) | 1:115:A:ILE:HD12 | 1:121:A:LEU:HG | 8 | 0.67 |
| (1,587) | 1:115:A:ILE:HD13 | 1:121:A:LEU:HG | 8 | 0.67 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 5 | 0.67 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 5 | 0.67 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 5 | 0.67 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 3 | 0.67 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 2 | 0.67 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 16 | 0.67 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 16 | 0.67 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 16 | 0.67 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD11 | 19 | 0.67 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD12 | 19 | 0.67 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD13 | 19 | 0.67 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 10 | 0.67 |
| (1,278) | 1:74:A:LEU:HD11 | 1:87:A:VAL:HB | 19 | 0.67 |
| (1,278) | 1:74:A:LEU:HD12 | 1:87:A:VAL:HB | 19 | 0.67 |
| (1,278) | 1:74:A:LEU:HD13 | 1:87:A:VAL:HB | 19 | 0.67 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 14 | 0.67 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 18 | 0.67 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 8 | 0.67 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 8 | 0.67 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 8 | 0.67 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 4 | 0.67 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 4 | 0.67 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 4 | 0.67 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 19 | 0.66 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 19 | 0.66 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 19 | 0.66 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 19 | 0.66 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 19 | 0.66 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 19 | 0.66 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 3 | 0.66 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 3 | 0.66 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 3 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 3 | 0.66 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 14 | 0.66 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 14 | 0.66 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 14 | 0.66 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 14 | 0.66 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 3 | 0.66 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 3 | 0.66 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 3 | 0.66 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 3 | 0.66 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 3 | 0.66 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 3 | 0.66 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 11 | 0.66 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 11 | 0.66 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 2 | 0.66 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 2 | 0.66 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 17 | 0.66 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 17 | 0.66 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 15 | 0.66 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 13 | 0.66 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 13 | 0.66 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 13 | 0.66 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 4 | 0.66 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 3 | 0.66 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 17 | 0.66 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 17 | 0.66 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 17 | 0.66 |
| (1,1039) | 1:80:A:ILE:HD11 | 1:83:A:TRP:H | 9 | 0.66 |
| (1,1039) | 1:80:A:ILE:HD12 | 1:83:A:TRP:H | 9 | 0.66 |
| (1,1039) | 1:80:A:ILE:HD13 | 1:83:A:TRP:H | 9 | 0.66 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 19 | 0.66 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 19 | 0.66 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 19 | 0.66 |
| (1,966) | 1:69:A:PRO:HB3 | 1:70:A:PHE:H | 19 | 0.66 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 19 | 0.66 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 19 | 0.66 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 19 | 0.66 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 9 | 0.66 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 1 | 0.66 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 11 | 0.66 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 11 | 0.66 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 11 | 0.66 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 2 | 0.66 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 2 | 0.66 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 2 | 0.66 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 6 | 0.66 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 6 | 0.66 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 6 | 0.66 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 11 | 0.66 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB1 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB2 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB3 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB1 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB2 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB3 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB1 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB2 | 14 | 0.66 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB3 | 14 | 0.66 |
| (1,229) | 1:69:A:PRO:HA | 1:128:A:LEU:HG | 7 | 0.66 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 6 | 0.66 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 18 | 0.66 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 13 | 0.66 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 18 | 0.66 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 1 | 0.66 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 1 | 0.66 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 1 | 0.66 |
| (1,106) | 1:45:A:LYS:H | 1:45:A:LYS:HE3 | 20 | 0.66 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 9 | 0.66 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 9 | 0.66 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 9 | 0.66 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 1 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 1 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 1 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 1 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 1 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 1 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 8 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 8 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 8 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 8 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 8 | 0.65 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 8 | 0.65 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 16 | 0.65 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 16 | 0.65 |
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 16 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 16 | 0.65 |
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 16 | 0.65 |
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 16 | 0.65 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 19 | 0.65 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 19 | 0.65 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 4 | 0.65 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 4 | 0.65 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 4 | 0.65 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 4 | 0.65 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 4 | 0.65 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 4 | 0.65 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG11 | 4 | 0.65 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG12 | 4 | 0.65 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG13 | 4 | 0.65 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG11 | 4 | 0.65 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG12 | 4 | 0.65 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG13 | 4 | 0.65 |
| (1,1332) | 1:24:A:ALA:HA | 1:103:A:GLN:HG2 | 18 | 0.65 |
| (1,1332) | 1:24:A:ALA:HA | 1:103:A:GLN:HG3 | 18 | 0.65 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 9 | 0.65 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 15 | 0.65 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 1 | 0.65 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 12 | 0.65 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 12 | 0.65 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 12 | 0.65 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 1 | 0.65 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 1 | 0.65 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 1 | 0.65 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 18 | 0.65 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 18 | 0.65 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 18 | 0.65 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 20 | 0.65 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 1 | 0.65 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 6 | 0.65 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 10 | 0.65 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 9 | 0.65 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 9 | 0.65 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 9 | 0.65 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 2 | 0.65 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 2 | 0.65 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 2 | 0.65 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 17 | 0.65 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 17 | 0.65 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 17 | 0.65 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 19 | 0.65 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 13 | 0.65 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 14 | 0.65 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 7 | 0.65 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 19 | 0.65 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 19 | 0.65 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 19 | 0.65 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 4 | 0.65 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 17 | 0.65 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 19 | 0.64 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 19 | 0.64 |
| (1,1475) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 3 | 0.64 |
| (1,1475) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 3 | 0.64 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 16 | 0.64 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 16 | 0.64 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 16 | 0.64 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 5 | 0.64 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 17 | 0.64 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 9 | 0.64 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 10 | 0.64 |
| (1,903) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 9 | 0.64 |
| (1,902) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 7 | 0.64 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 7 | 0.64 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 8 | 0.64 |
| (1,800) | 1:41:A:GLN:H | 1:44:A:LYS:HB2 | 20 | 0.64 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 15 | 0.64 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 2 | 0.64 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 12 | 0.64 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 1 | 0.64 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 1 | 0.64 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 1 | 0.64 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 14 | 0.64 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 14 | 0.64 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 14 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 6 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 6 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 7 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 8 | 0.64 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 8 | 0.64 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 2 | 0.64 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 2 | 0.64 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 2 | 0.64 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 9 | 0.64 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 12 | 0.64 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 19 | 0.64 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 13 | 0.63 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 13 | 0.63 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 13 | 0.63 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 13 | 0.63 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 13 | 0.63 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 13 | 0.63 |
| (1,1405) | 1:44:A:LYS:HE2 | 1:45:A:LYS:H | 15 | 0.63 |
| (1,1405) | 1:44:A:LYS:HE3 | 1:45:A:LYS:H | 15 | 0.63 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 5 | 0.63 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 5 | 0.63 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 5 | 0.63 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 5 | 0.63 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG11 | 20 | 0.63 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG12 | 20 | 0.63 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG13 | 20 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG11 | 20 | 0.63 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG12 | 20 | 0.63 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG13 | 20 | 0.63 |
| (1,1308) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 8 | 0.63 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 2 | 0.63 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 2 | 0.63 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 2 | 0.63 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 16 | 0.63 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 16 | 0.63 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 16 | 0.63 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 11 | 0.63 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 12 | 0.63 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 19 | 0.63 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 19 | 0.63 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 19 | 0.63 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 2 | 0.63 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 10 | 0.63 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 18 | 0.63 |
| (1,689) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD1 | 3 | 0.63 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 11 | 0.63 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 11 | 0.63 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 11 | 0.63 |
| (1,644) | 1:49:A:HIS:HB2 | 1:128:A:LEU:HG | 5 | 0.63 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 12 | 0.63 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 12 | 0.63 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 12 | 0.63 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 13 | 0.63 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 10 | 0.63 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 10 | 0.63 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 10 | 0.63 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 5 | 0.63 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 5 | 0.63 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 5 | 0.63 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 14 | 0.63 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 14 | 0.63 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 14 | 0.63 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 10 | 0.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 10 | 0.63 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 19 | 0.63 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 19 | 0.63 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG21 | 4 | 0.63 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG22 | 4 | 0.63 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG23 | 4 | 0.63 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 13 | 0.63 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 9 | 0.63 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 14 | 0.63 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 14 | 0.63 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 18 | 0.63 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 17 | 0.63 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 17 | 0.63 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 17 | 0.63 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG11 | 8 | 0.63 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG12 | 8 | 0.63 |
| (1,59) | 1:38:A:THR:HA | 1:130:A:VAL:HG13 | 8 | 0.63 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 15 | 0.63 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 17 | 0.62 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 17 | 0.62 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 17 | 0.62 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 17 | 0.62 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 17 | 0.62 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 17 | 0.62 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 7 | 0.62 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 7 | 0.62 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 7 | 0.62 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 7 | 0.62 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 7 | 0.62 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 7 | 0.62 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 4 | 0.62 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 4 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG11 | 11 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG12 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG13 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG21 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG22 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG23 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG11 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG12 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG13 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG21 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG22 | 11 | 0.62 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG23 | 11 | 0.62 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 1 | 0.62 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 8 | 0.62 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 5 | 0.62 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 5 | 0.62 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 5 | 0.62 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 6 | 0.62 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 14 | 0.62 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD11 | 19 | 0.62 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD12 | 19 | 0.62 |
| (1,568) | 1:111:A:TYR:H | 1:115:A:ILE:HD13 | 19 | 0.62 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 1 | 0.62 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 19 | 0.62 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 19 | 0.62 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 19 | 0.62 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 6 | 0.62 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 17 | 0.62 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 3 | 0.62 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 15 | 0.62 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 17 | 0.62 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 3 | 0.62 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 3 | 0.62 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 3 | 0.62 |
| (1,106) | 1:45:A:LYS:H | 1:45:A:LYS:HE3 | 10 | 0.62 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 10 | 0.62 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 10 | 0.62 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 10 | 0.62 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 8 | 0.62 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 6 | 0.62 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 14 | 0.62 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 14 | 0.62 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 14 | 0.62 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 4 | 0.62 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 19 | 0.62 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 12 | 0.62 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 15 | 0.62 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 17 | 0.61 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 17 | 0.61 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 17 | 0.61 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 17 | 0.61 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 17 | 0.61 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 17 | 0.61 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 2 | 0.61 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 2 | 0.61 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 2 | 0.61 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 2 | 0.61 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 2 | 0.61 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 2 | 0.61 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 13 | 0.61 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 13 | 0.61 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 4 | 0.61 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 4 | 0.61 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 4 | 0.61 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 4 | 0.61 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 4 | 0.61 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 4 | 0.61 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 14 | 0.61 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 14 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 19 | 0.61 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 19 | 0.61 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 18 | 0.61 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 18 | 0.61 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 18 | 0.61 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 18 | 0.61 |
| (1,1325) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 2 | 0.61 |
| (1,1325) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 2 | 0.61 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 7 | 0.61 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 3 | 0.61 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 3 | 0.61 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 3 | 0.61 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 14 | 0.61 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 16 | 0.61 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 16 | 0.61 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 16 | 0.61 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 12 | 0.61 |
| (1,1049) | 1:81:A:LYS:HD3 | 1:84:A:ASP:H | 19 | 0.61 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 15 | 0.61 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 15 | 0.61 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 15 | 0.61 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 4 | 0.61 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 4 | 0.61 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 4 | 0.61 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 8 | 0.61 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 8 | 0.61 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 8 | 0.61 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 17 | 0.61 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 3 | 0.61 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 3 | 0.61 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 3 | 0.61 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 3 | 0.61 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 16 | 0.61 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 20 | 0.61 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 6 | 0.61 |
| (1,543) | 1:108:A:GLU:HA | 1:118:A:LYS:HG2 | 3 | 0.61 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 3 | 0.61 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 10 | 0.61 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 8 | 0.61 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 11 | 0.61 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 11 | 0.61 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 11 | 0.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 3 | 0.61 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 20 | 0.61 |
| (1,234) | 1:69:A:PRO:HB3 | 1:128:A:LEU:HG | 7 | 0.61 |
| (1,200) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 16 | 0.61 |
| (1,190) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD2 | 11 | 0.61 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 18 | 0.61 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 6 | 0.61 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 6 | 0.61 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 6 | 0.61 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 14 | 0.61 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 6 | 0.61 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 6 | 0.61 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 6 | 0.61 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 2 | 0.61 |
| (1,1624) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 6 | 0.6 |
| (1,1624) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 6 | 0.6 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 15 | 0.6 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 15 | 0.6 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 15 | 0.6 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 15 | 0.6 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 15 | 0.6 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 15 | 0.6 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 20 | 0.6 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 20 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 6 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 6 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 6 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 6 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 6 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 6 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 7 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 7 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 7 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 7 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 7 | 0.6 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 7 | 0.6 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 1 | 0.6 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 1 | 0.6 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 1 | 0.6 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 1 | 0.6 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 10 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 10 | 0.6 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 10 | 0.6 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 15 | 0.6 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 15 | 0.6 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 2 | 0.6 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 2 | 0.6 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 15 | 0.6 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 5 | 0.6 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 14 | 0.6 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 11 | 0.6 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 11 | 0.6 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 11 | 0.6 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 1 | 0.6 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 1 | 0.6 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 1 | 0.6 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 13 | 0.6 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 13 | 0.6 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 13 | 0.6 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 1 | 0.6 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 10 | 0.6 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 15 | 0.6 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 15 | 0.6 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 15 | 0.6 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 18 | 0.6 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 18 | 0.6 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 18 | 0.6 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 17 | 0.6 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 9 | 0.6 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 6 | 0.6 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 8 | 0.6 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 13 | 0.6 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 2 | 0.6 |
| (1,292) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HG2 | 11 | 0.6 |
| (1,292) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HG2 | 11 | 0.6 |
| (1,292) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HG2 | 11 | 0.6 |
| (1,271) | 1:74:A:LEU:HD21 | 1:88:A:ALA:H | 11 | 0.6 |
| (1,271) | 1:74:A:LEU:HD22 | 1:88:A:ALA:H | 11 | 0.6 |
| (1,271) | 1:74:A:LEU:HD23 | 1:88:A:ALA:H | 11 | 0.6 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 8 | 0.6 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 14 | 0.6 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 14 | 0.6 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 14 | 0.6 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 20 | 0.6 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 15 | 0.6 |
| (1,153) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 17 | 0.6 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 12 | 0.6 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 12 | 0.6 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 12 | 0.6 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 1 | 0.6 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 11 | 0.59 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 11 | 0.59 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 18 | 0.59 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 18 | 0.59 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 18 | 0.59 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 18 | 0.59 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 16 | 0.59 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 16 | 0.59 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB2 | 13 | 0.59 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB3 | 13 | 0.59 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 5 | 0.59 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 5 | 0.59 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 5 | 0.59 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 5 | 0.59 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 5 | 0.59 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 5 | 0.59 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 6 | 0.59 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 6 | 0.59 |
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 20 | 0.59 |
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 20 | 0.59 |
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 20 | 0.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 20 | 0.59 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 9 | 0.59 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 9 | 0.59 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 8 | 0.59 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 18 | 0.59 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 18 | 0.59 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 18 | 0.59 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 10 | 0.59 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 2 | 0.59 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 2 | 0.59 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 2 | 0.59 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 14 | 0.59 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 16 | 0.59 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 14 | 0.59 |
| (1,457) | 1:29:A:LYS:H | 1:97:A:LEU:HB2 | 7 | 0.59 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 16 | 0.59 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 16 | 0.59 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 16 | 0.59 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 6 | 0.59 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 6 | 0.59 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 6 | 0.59 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 18 | 0.59 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 18 | 0.59 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 18 | 0.59 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD11 | 9 | 0.59 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD12 | 9 | 0.59 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD13 | 9 | 0.59 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 18 | 0.59 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 18 | 0.59 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 18 | 0.59 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 14 | 0.59 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 14 | 0.59 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 14 | 0.59 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 1 | 0.58 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 1 | 0.58 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 1 | 0.58 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 1 | 0.58 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 1 | 0.58 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 1 | 0.58 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 8 | 0.58 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 8 | 0.58 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 3 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 3 | 0.58 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 11 | 0.58 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 11 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG11 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG12 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG13 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG21 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG22 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG23 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG11 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG12 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG13 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG21 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG22 | 10 | 0.58 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG23 | 10 | 0.58 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 13 | 0.58 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 13 | 0.58 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 17 | 0.58 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 17 | 0.58 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 18 | 0.58 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 18 | 0.58 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 6 | 0.58 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 6 | 0.58 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 6 | 0.58 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 4 | 0.58 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 4 | 0.58 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 4 | 0.58 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 19 | 0.58 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 18 | 0.58 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 10 | 0.58 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 2 | 0.58 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 2 | 0.58 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 2 | 0.58 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 16 | 0.58 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 2 | 0.58 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 11 | 0.58 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 19 | 0.58 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 2 | 0.58 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 2 | 0.58 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 2 | 0.58 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 19 | 0.58 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 19 | 0.58 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 19 | 0.58 |
| (1,587) | 1:115:A:ILE:HD11 | 1:121:A:LEU:HG | 5 | 0.58 |
| (1,587) | 1:115:A:ILE:HD12 | 1:121:A:LEU:HG | 5 | 0.58 |
| (1,587) | 1:115:A:ILE:HD13 | 1:121:A:LEU:HG | 5 | 0.58 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 19 | 0.58 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 7 | 0.58 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 14 | 0.58 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 9 | 0.58 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 9 | 0.58 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 9 | 0.58 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 15 | 0.58 |
| (1,343) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 9 | 0.58 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 16 | 0.58 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 16 | 0.58 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 16 | 0.58 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 5 | 0.58 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 8 | 0.58 |
| (1,183) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 1 | 0.58 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 2 | 0.58 |
| (1,176) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG3 | 2 | 0.58 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 19 | 0.58 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 12 | 0.58 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 16 | 0.58 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 4 | 0.58 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 20 | 0.58 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 20 | 0.58 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 20 | 0.58 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 17 | 0.58 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 17 | 0.58 |
| (1,1619) | 1:103:A:GLN:HG2 | 1:104:A:LEU:H | 11 | 0.57 |
| (1,1619) | 1:103:A:GLN:HG3 | 1:104:A:LEU:H | 11 | 0.57 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 3 | 0.57 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 3 | 0.57 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 20 | 0.57 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 20 | 0.57 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 20 | 0.57 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 20 | 0.57 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 20 | 0.57 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 20 | 0.57 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 13 | 0.57 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 13 | 0.57 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 13 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 13 | 0.57 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 13 | 0.57 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 13 | 0.57 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG2 | 11 | 0.57 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG3 | 11 | 0.57 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG2 | 11 | 0.57 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG3 | 11 | 0.57 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG2 | 11 | 0.57 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG3 | 11 | 0.57 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 3 | 0.57 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 3 | 0.57 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 17 | 0.57 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 17 | 0.57 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 17 | 0.57 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 17 | 0.57 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 6 | 0.57 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 6 | 0.57 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 6 | 0.57 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 12 | 0.57 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 12 | 0.57 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 12 | 0.57 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 10 | 0.57 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 14 | 0.57 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 1 | 0.57 |
| (1,910) | 1:55:A:PRO:HA | 1:57:A:GLY:H | 17 | 0.57 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 13 | 0.57 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 14 | 0.57 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 14 | 0.57 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 14 | 0.57 |
| (1,692) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HD1 | 14 | 0.57 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 8 | 0.57 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 8 | 0.57 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 8 | 0.57 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 20 | 0.57 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 14 | 0.57 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 3 | 0.57 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 12 | 0.57 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 12 | 0.57 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 11 | 0.57 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 12 | 0.57 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 12 | 0.57 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 12 | 0.57 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 3 | 0.57 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 3 | 0.57 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 3 | 0.57 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 9 | 0.57 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 10 | 0.57 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 1 | 0.57 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 5 | 0.57 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 2 | 0.57 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 2 | 0.57 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 2 | 0.57 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 10 | 0.57 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 10 | 0.57 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 10 | 0.57 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 3 | 0.57 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 3 | 0.57 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 3 | 0.57 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG21 | 7 | 0.57 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG22 | 7 | 0.57 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG23 | 7 | 0.57 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG21 | 7 | 0.57 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG22 | 7 | 0.57 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG23 | 7 | 0.57 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 12 | 0.57 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 11 | 0.57 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 6 | 0.56 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 6 | 0.56 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 16 | 0.56 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 16 | 0.56 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 16 | 0.56 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 16 | 0.56 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 16 | 0.56 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 16 | 0.56 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 18 | 0.56 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 18 | 0.56 |
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 2 | 0.56 |
| (1,1476) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 2 | 0.56 |
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 2 | 0.56 |
| (1,1476) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 2 | 0.56 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 8 | 0.56 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 8 | 0.56 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 8 | 0.56 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 8 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 8 | 0.56 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 8 | 0.56 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 2 | 0.56 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 2 | 0.56 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 2 | 0.56 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 2 | 0.56 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 2 | 0.56 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 2 | 0.56 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 11 | 0.56 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 11 | 0.56 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 18 | 0.56 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 18 | 0.56 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 18 | 0.56 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 18 | 0.56 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 18 | 0.56 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 18 | 0.56 |
| (1,1308) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 19 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 7 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 7 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 7 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 9 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 9 | 0.56 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 9 | 0.56 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 12 | 0.56 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 12 | 0.56 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 12 | 0.56 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 8 | 0.56 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 4 | 0.56 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 17 | 0.56 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 17 | 0.56 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 17 | 0.56 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 7 | 0.56 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 2 | 0.56 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 2 | 0.56 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 2 | 0.56 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 16 | 0.56 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 16 | 0.56 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 16 | 0.56 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 8 | 0.56 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 13 | 0.56 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 13 | 0.56 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 13 | 0.56 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 5 | 0.56 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 5 | 0.56 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 5 | 0.56 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 18 | 0.56 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 16 | 0.56 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 16 | 0.56 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 16 | 0.56 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 18 | 0.56 |
| (1,575) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HG2 | 17 | 0.56 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 12 | 0.56 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 12 | 0.56 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 12 | 0.56 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 5 | 0.56 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 14 | 0.56 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 14 | 0.56 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 14 | 0.56 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 2 | 0.56 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 2 | 0.56 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 2 | 0.56 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 2 | 0.56 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 14 | 0.56 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 14 | 0.56 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 14 | 0.56 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 17 | 0.56 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 9 | 0.56 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 18 | 0.56 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 12 | 0.56 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 6 | 0.56 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 9 | 0.56 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 13 | 0.56 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 17 | 0.56 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 17 | 0.56 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 9 | 0.56 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 10 | 0.55 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 10 | 0.55 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 9 | 0.55 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 9 | 0.55 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 4 | 0.55 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 4 | 0.55 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 13 | 0.55 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 18 | 0.55 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 9 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 12 | 0.55 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 12 | 0.55 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 12 | 0.55 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 13 | 0.55 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 13 | 0.55 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 13 | 0.55 |
| (1,952) | 1:67:A:GLY:H | 1:68:A:LYS:HB2 | 18 | 0.55 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 9 | 0.55 |
| (1,800) | 1:41:A:GLN:H | 1:44:A:LYS:HB2 | 3 | 0.55 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 2 | 0.55 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 2 | 0.55 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 2 | 0.55 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG21 | 12 | 0.55 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG22 | 12 | 0.55 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG23 | 12 | 0.55 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 8 | 0.55 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 7 | 0.55 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 7 | 0.55 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 7 | 0.55 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 9 | 0.55 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 9 | 0.55 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 9 | 0.55 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 13 | 0.55 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 13 | 0.55 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 13 | 0.55 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 6 | 0.55 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 10 | 0.55 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 4 | 0.55 |
| (1,623) | 1:95:A:LYS:HB2 | 1:126:A:GLU:HA | 9 | 0.55 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 8 | 0.55 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 13 | 0.55 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 13 | 0.55 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 13 | 0.55 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 4 | 0.55 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 4 | 0.55 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 4 | 0.55 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 17 | 0.55 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 4 | 0.55 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 4 | 0.55 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 4 | 0.55 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 4 | 0.55 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 4 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 4 | 0.55 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 4 | 0.55 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 4 | 0.55 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 4 | 0.55 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 11 | 0.55 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 17 | 0.55 |
| (1,354) | 1:82:A:GLY:HA2 | 1:104:A:LEU:HB3 | 1 | 0.55 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 12 | 0.55 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 12 | 0.55 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 12 | 0.55 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 17 | 0.55 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 17 | 0.55 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 17 | 0.55 |
| (1,278) | 1:74:A:LEU:HD11 | 1:87:A:VAL:HB | 6 | 0.55 |
| (1,278) | 1:74:A:LEU:HD12 | 1:87:A:VAL:HB | 6 | 0.55 |
| (1,278) | 1:74:A:LEU:HD13 | 1:87:A:VAL:HB | 6 | 0.55 |
| (1,271) | 1:74:A:LEU:HD21 | 1:88:A:ALA:H | 4 | 0.55 |
| (1,271) | 1:74:A:LEU:HD22 | 1:88:A:ALA:H | 4 | 0.55 |
| (1,271) | 1:74:A:LEU:HD23 | 1:88:A:ALA:H | 4 | 0.55 |
| (1,201) | 1:59:A:GLN:H | 1:59:A:GLN:HG3 | 17 | 0.55 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 13 | 0.55 |
| (1,145) | 1:49:A:HIS:HB2 | 1:126:A:GLU:HG2 | 16 | 0.55 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 7 | 0.54 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 7 | 0.54 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 7 | 0.54 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 7 | 0.54 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 7 | 0.54 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 7 | 0.54 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 2 | 0.54 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 2 | 0.54 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 2 | 0.54 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 2 | 0.54 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 2 | 0.54 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 2 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG11 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG12 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG13 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG21 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG22 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG23 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG11 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG12 | 16 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG13 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG21 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG22 | 16 | 0.54 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG23 | 16 | 0.54 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 18 | 0.54 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 18 | 0.54 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 18 | 0.54 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 3 | 0.54 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 6 | 0.54 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 15 | 0.54 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 5 | 0.54 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 5 | 0.54 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 5 | 0.54 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 10 | 0.54 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 10 | 0.54 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 10 | 0.54 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 4 | 0.54 |
| (1,797) | 1:41:A:GLN:H | 1:41:A:GLN:HG2 | 8 | 0.54 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 5 | 0.54 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 5 | 0.54 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 5 | 0.54 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 6 | 0.54 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 3 | 0.54 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 13 | 0.54 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 13 | 0.54 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 13 | 0.54 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 13 | 0.54 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG21 | 12 | 0.54 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG22 | 12 | 0.54 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG23 | 12 | 0.54 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG21 | 19 | 0.54 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG22 | 19 | 0.54 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG23 | 19 | 0.54 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 10 | 0.54 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 10 | 0.54 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 10 | 0.54 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 4 | 0.54 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 6 | 0.54 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 15 | 0.54 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 14 | 0.54 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 5 | 0.54 |
| (1,481) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HA | 4 | 0.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,481) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HA | 4 | 0.54 |
| (1,481) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HA | 4 | 0.54 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 4 | 0.54 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 4 | 0.54 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 4 | 0.54 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 7 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 1 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 1 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 1 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 13 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 13 | 0.54 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 13 | 0.54 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 4 | 0.54 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 12 | 0.54 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 9 | 0.54 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 9 | 0.54 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 9 | 0.54 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 8 | 0.54 |
| (1,92) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 4 | 0.54 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 20 | 0.54 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 20 | 0.54 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 20 | 0.54 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 7 | 0.54 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 7 | 0.54 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 7 | 0.54 |
| (1,62) | 1:38:A:THR:HB | 1:92:A:LEU:H | 7 | 0.54 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 11 | 0.53 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 11 | 0.53 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 11 | 0.53 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 11 | 0.53 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 11 | 0.53 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 11 | 0.53 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 20 | 0.53 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 20 | 0.53 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 20 | 0.53 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 20 | 0.53 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 20 | 0.53 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 20 | 0.53 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 9 | 0.53 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 9 | 0.53 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 13 | 0.53 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 13 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 13 | 0.53 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 13 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG11 | 6 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG12 | 6 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG13 | 6 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG11 | 6 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG12 | 6 | 0.53 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG13 | 6 | 0.53 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 14 | 0.53 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 14 | 0.53 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 16 | 0.53 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 16 | 0.53 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 16 | 0.53 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 2 | 0.53 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 2 | 0.53 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 2 | 0.53 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 20 | 0.53 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 15 | 0.53 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 7 | 0.53 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 12 | 0.53 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 12 | 0.53 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 18 | 0.53 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG21 | 19 | 0.53 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG22 | 19 | 0.53 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG23 | 19 | 0.53 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 20 | 0.53 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 20 | 0.53 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 20 | 0.53 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG11 | 4 | 0.53 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG12 | 4 | 0.53 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG13 | 4 | 0.53 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 6 | 0.53 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 6 | 0.53 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 6 | 0.53 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 6 | 0.53 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 6 | 0.53 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 6 | 0.53 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 6 | 0.53 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 20 | 0.53 |
| (1,443) | 1:32:A:THR:HG21 | 1:95:A:LYS:HB3 | 1 | 0.53 |
| (1,443) | 1:32:A:THR:HG22 | 1:95:A:LYS:HB3 | 1 | 0.53 |
| (1,443) | 1:32:A:THR:HG23 | 1:95:A:LYS:HB3 | 1 | 0.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,417) | 1:90:A:MET:HE1 | 1:94:A:GLU:HG2 | 14 | 0.53 |
| (1,417) | 1:90:A:MET:HE2 | 1:94:A:GLU:HG2 | 14 | 0.53 |
| (1,417) | 1:90:A:MET:HE3 | 1:94:A:GLU:HG2 | 14 | 0.53 |
| (1,394) | 1:74:A:LEU:HD11 | 1:88:A:ALA:HA | 9 | 0.53 |
| (1,394) | 1:74:A:LEU:HD12 | 1:88:A:ALA:HA | 9 | 0.53 |
| (1,394) | 1:74:A:LEU:HD13 | 1:88:A:ALA:HA | 9 | 0.53 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 17 | 0.53 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 20 | 0.53 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 15 | 0.53 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 17 | 0.53 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 17 | 0.53 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 17 | 0.53 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 20 | 0.53 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 20 | 0.53 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 20 | 0.53 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 5 | 0.53 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 20 | 0.53 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 17 | 0.53 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 8 | 0.53 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 8 | 0.53 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 8 | 0.53 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 1 | 0.53 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 8 | 0.53 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 8 | 0.53 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 8 | 0.53 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 8 | 0.53 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 2 | 0.53 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 1 | 0.53 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 1 | 0.53 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 1 | 0.53 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 1 | 0.52 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 1 | 0.52 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 1 | 0.52 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 1 | 0.52 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 1 | 0.52 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 1 | 0.52 |
| (1,1619) | 1:103:A:GLN:HG2 | 1:104:A:LEU:H | 19 | 0.52 |
| (1,1619) | 1:103:A:GLN:HG3 | 1:104:A:LEU:H | 19 | 0.52 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 2 | 0.52 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 2 | 0.52 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 2 | 0.52 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 2 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 2 | 0.52 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 2 | 0.52 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 8 | 0.52 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 8 | 0.52 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 8 | 0.52 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 8 | 0.52 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 8 | 0.52 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 8 | 0.52 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 4 | 0.52 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 4 | 0.52 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 4 | 0.52 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 4 | 0.52 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 4 | 0.52 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 4 | 0.52 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 9 | 0.52 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 9 | 0.52 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 9 | 0.52 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 9 | 0.52 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 9 | 0.52 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 9 | 0.52 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 9 | 0.52 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 9 | 0.52 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 14 | 0.52 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 14 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 18 | 0.52 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 18 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 20 | 0.52 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 20 | 0.52 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 20 | 0.52 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 20 | 0.52 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 20 | 0.52 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 20 | 0.52 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 14 | 0.52 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 14 | 0.52 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 14 | 0.52 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 9 | 0.52 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 14 | 0.52 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 2 | 0.52 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 2 | 0.52 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 2 | 0.52 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 4 | 0.52 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 4 | 0.52 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 4 | 0.52 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 6 | 0.52 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 16 | 0.52 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 2 | 0.52 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 6 | 0.52 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 8 | 0.52 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 6 | 0.52 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG21 | 15 | 0.52 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG22 | 15 | 0.52 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG23 | 15 | 0.52 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 15 | 0.52 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 15 | 0.52 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 15 | 0.52 |
| (1,651) | 1:92:A:LEU:HD11 | 1:129:A:ALA:HA | 10 | 0.52 |
| (1,651) | 1:92:A:LEU:HD12 | 1:129:A:ALA:HA | 10 | 0.52 |
| (1,651) | 1:92:A:LEU:HD13 | 1:129:A:ALA:HA | 10 | 0.52 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 6 | 0.52 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 16 | 0.52 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 15 | 0.52 |
| (1,457) | 1:29:A:LYS:H | 1:97:A:LEU:HB2 | 3 | 0.52 |
| (1,450) | 1:32:A:THR:HB | 1:95:A:LYS:HE3 | 10 | 0.52 |
| (1,358) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HB2 | 9 | 0.52 |
| (1,358) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HB2 | 9 | 0.52 |
| (1,358) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HB2 | 9 | 0.52 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 7 | 0.52 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 7 | 0.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 7 | 0.52 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 5 | 0.52 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 5 | 0.52 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 14 | 0.52 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG21 | 17 | 0.52 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG22 | 17 | 0.52 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG23 | 17 | 0.52 |
| (1,159) | 1:53:A:ARG:HB2 | 1:59:A:GLN:H | 20 | 0.52 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 4 | 0.52 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 14 | 0.52 |
| (1,1656) | 1:126:A:GLU:HB2 | 1:128:A:LEU:HD11 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB2 | 1:128:A:LEU:HD12 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB2 | 1:128:A:LEU:HD13 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB2 | 1:128:A:LEU:HD21 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB2 | 1:128:A:LEU:HD22 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB2 | 1:128:A:LEU:HD23 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB3 | 1:128:A:LEU:HD11 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB3 | 1:128:A:LEU:HD12 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB3 | 1:128:A:LEU:HD13 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB3 | 1:128:A:LEU:HD21 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB3 | 1:128:A:LEU:HD22 | 9 | 0.51 |
| (1,1656) | 1:126:A:GLU:HB3 | 1:128:A:LEU:HD23 | 9 | 0.51 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 16 | 0.51 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 16 | 0.51 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 16 | 0.51 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 16 | 0.51 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 16 | 0.51 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 16 | 0.51 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 10 | 0.51 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 10 | 0.51 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 10 | 0.51 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 10 | 0.51 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 10 | 0.51 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 10 | 0.51 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 2 | 0.51 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 2 | 0.51 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 19 | 0.51 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 19 | 0.51 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 7 | 0.51 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 7 | 0.51 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 12 | 0.51 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 12 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 11 | 0.51 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 11 | 0.51 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 11 | 0.51 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 11 | 0.51 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 18 | 0.51 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 18 | 0.51 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 18 | 0.51 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 3 | 0.51 |
| (1,1162) | 1:27:A:GLU:HB2 | 1:99:A:THR:H | 18 | 0.51 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 4 | 0.51 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 15 | 0.51 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 9 | 0.51 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 2 | 0.51 |
| (1,966) | 1:69:A:PRO:HB3 | 1:70:A:PHE:H | 1 | 0.51 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 18 | 0.51 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 1 | 0.51 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 13 | 0.51 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 1 | 0.51 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 1 | 0.51 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 1 | 0.51 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 12 | 0.51 |
| (1,608) | 1:97:A:LEU:HG | 1:124:A:GLU:HG3 | 9 | 0.51 |
| (1,601) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB2 | 9 | 0.51 |
| (1,601) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB2 | 9 | 0.51 |
| (1,601) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB2 | 9 | 0.51 |
| (1,545) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 16 | 0.51 |
| (1,543) | 1:108:A:GLU:HA | 1:118:A:LYS:HG2 | 14 | 0.51 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 3 | 0.51 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 3 | 0.51 |
| (1,524) | 1:80:A:ILE:HD11 | 1:105:A:ALA:HB1 | 9 | 0.51 |
| (1,524) | 1:80:A:ILE:HD11 | 1:105:A:ALA:HB2 | 9 | 0.51 |
| (1,524) | 1:80:A:ILE:HD11 | 1:105:A:ALA:HB3 | 9 | 0.51 |
| (1,524) | 1:80:A:ILE:HD12 | 1:105:A:ALA:HB1 | 9 | 0.51 |
| (1,524) | 1:80:A:ILE:HD12 | 1:105:A:ALA:HB2 | 9 | 0.51 |
| (1,524) | 1:80:A:ILE:HD12 | 1:105:A:ALA:HB3 | 9 | 0.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,524) | 1:80:A:ILE:HD13 | 1:105:A:ALA:HB1 | 9 | 0.51 |
| (1,524) | 1:80:A:ILE:HD13 | 1:105:A:ALA:HB2 | 9 | 0.51 |
| (1,524) | 1:80:A:ILE:HD13 | 1:105:A:ALA:HB3 | 9 | 0.51 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 2 | 0.51 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 13 | 0.51 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 13 | 0.51 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 13 | 0.51 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 19 | 0.51 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 19 | 0.51 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 19 | 0.51 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 1 | 0.51 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 1 | 0.51 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 1 | 0.51 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 14 | 0.51 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 18 | 0.51 |
| (1,200) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 20 | 0.51 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 20 | 0.51 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 20 | 0.51 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 20 | 0.51 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 9 | 0.51 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 9 | 0.51 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 9 | 0.51 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 9 | 0.51 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 9 | 0.51 |
| (1,20) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 6 | 0.51 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 16 | 0.5 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 16 | 0.5 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB2 | 10 | 0.5 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB3 | 10 | 0.5 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 6 | 0.5 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 6 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG11 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG12 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG13 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG21 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG22 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB2 | 1:130:A:VAL:HG23 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG11 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG12 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG13 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG21 | 10 | 0.5 |
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG22 | 10 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1383) | 1:40:A:PRO:HB3 | 1:130:A:VAL:HG23 | 10 | 0.5 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 17 | 0.5 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 17 | 0.5 |
| (1,1204) | 1:100:A:ILE:HG21 | 1:106:A:TYR:H | 7 | 0.5 |
| (1,1204) | 1:100:A:ILE:HG22 | 1:106:A:TYR:H | 7 | 0.5 |
| (1,1204) | 1:100:A:ILE:HG23 | 1:106:A:TYR:H | 7 | 0.5 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 7 | 0.5 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 7 | 0.5 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 1 | 0.5 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 17 | 0.5 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 14 | 0.5 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 17 | 0.5 |
| (1,929) | 1:63:A:SER:H | 1:64:A:ARG:HG3 | 17 | 0.5 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 5 | 0.5 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 11 | 0.5 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 2 | 0.5 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 17 | 0.5 |
| (1,689) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD1 | 1 | 0.5 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 3 | 0.5 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 3 | 0.5 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 3 | 0.5 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 17 | 0.5 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 20 | 0.5 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 8 | 0.5 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 8 | 0.5 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 8 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 14 | 0.5 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 14 | 0.5 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 14 | 0.5 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 12 | 0.5 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 12 | 0.5 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 12 | 0.5 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD21 | 15 | 0.5 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD22 | 15 | 0.5 |
| (1,508) | 1:80:A:ILE:HA | 1:104:A:LEU:HD23 | 15 | 0.5 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 9 | 0.5 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 9 | 0.5 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 9 | 0.5 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 3 | 0.5 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 3 | 0.5 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 3 | 0.5 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 19 | 0.5 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 19 | 0.5 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 19 | 0.5 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 3 | 0.5 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 3 | 0.5 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 3 | 0.5 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 10 | 0.5 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 9 | 0.5 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 9 | 0.5 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 9 | 0.5 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 3 | 0.5 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 3 | 0.5 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 3 | 0.5 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 2 | 0.5 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 2 | 0.5 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 2 | 0.5 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 15 | 0.5 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 15 | 0.5 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 15 | 0.5 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 9 | 0.5 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 7 | 0.5 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 10 | 0.5 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 10 | 0.5 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 10 | 0.5 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 10 | 0.5 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 10 | 0.5 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 10 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 10 | 0.5 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 10 | 0.5 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 10 | 0.5 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 1 | 0.49 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 1 | 0.49 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 1 | 0.49 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 1 | 0.49 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 1 | 0.49 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 1 | 0.49 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 8 | 0.49 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 8 | 0.49 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 8 | 0.49 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 8 | 0.49 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 8 | 0.49 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 8 | 0.49 |
| (1,1584) | 1:95:A:LYS:HG2 | 1:124:A:GLU:HB3 | 9 | 0.49 |
| (1,1584) | 1:95:A:LYS:HG3 | 1:124:A:GLU:HB3 | 9 | 0.49 |
| (1,1575) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 3 | 0.49 |
| (1,1575) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 3 | 0.49 |
| (1,1575) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 3 | 0.49 |
| (1,1575) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 3 | 0.49 |
| (1,1575) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 3 | 0.49 |
| (1,1575) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 3 | 0.49 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 9 | 0.49 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 9 | 0.49 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 6 | 0.49 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 6 | 0.49 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 12 | 0.49 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 12 | 0.49 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 20 | 0.49 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 20 | 0.49 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 1 | 0.49 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 1 | 0.49 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 19 | 0.49 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 19 | 0.49 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 17 | 0.49 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 17 | 0.49 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 4 | 0.49 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 4 | 0.49 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 8 | 0.49 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 8 | 0.49 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 5 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 5 | 0.49 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 8 | 0.49 |
| (1,1306) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE21 | 4 | 0.49 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 5 | 0.49 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 5 | 0.49 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 5 | 0.49 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 7 | 0.49 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 3 | 0.49 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 1 | 0.49 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 16 | 0.49 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 16 | 0.49 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 16 | 0.49 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 5 | 0.49 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 5 | 0.49 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 5 | 0.49 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 15 | 0.49 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 13 | 0.49 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 17 | 0.49 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 2 | 0.49 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 4 | 0.49 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 19 | 0.49 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 9 | 0.49 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 9 | 0.49 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 9 | 0.49 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG11 | 4 | 0.49 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG12 | 4 | 0.49 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG13 | 4 | 0.49 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 9 | 0.49 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 3 | 0.49 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 9 | 0.49 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 10 | 0.49 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 6 | 0.49 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 6 | 0.49 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG21 | 18 | 0.49 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG22 | 18 | 0.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG23 | 18 | 0.49 |
| (1,449) | 1:32:A:THR:HB | 1:95:A:LYS:HE2 | 10 | 0.49 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 16 | 0.49 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 9 | 0.49 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 9 | 0.49 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 9 | 0.49 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB1 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB2 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD21 | 1:88:A:ALA:HB3 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB1 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB2 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD22 | 1:88:A:ALA:HB3 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB1 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB2 | 7 | 0.49 |
| (1,400) | 1:74:A:LEU:HD23 | 1:88:A:ALA:HB3 | 7 | 0.49 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 2 | 0.49 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 2 | 0.49 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 2 | 0.49 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 16 | 0.49 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 11 | 0.49 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 11 | 0.49 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 11 | 0.49 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 7 | 0.49 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 7 | 0.49 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 7 | 0.49 |
| (1,266) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 4 | 0.49 |
| (1,266) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 4 | 0.49 |
| (1,266) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 4 | 0.49 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 20 | 0.49 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 3 | 0.49 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 8 | 0.49 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 9 | 0.49 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 9 | 0.49 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 9 | 0.49 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG21 | 12 | 0.49 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG22 | 12 | 0.49 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG23 | 12 | 0.49 |
| (1,1624) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 13 | 0.48 |
| (1,1624) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 13 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 19 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 19 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 19 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 19 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 19 | 0.48 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 19 | 0.48 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 15 | 0.48 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 15 | 0.48 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 15 | 0.48 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 15 | 0.48 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 15 | 0.48 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 15 | 0.48 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 17 | 0.48 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 17 | 0.48 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 11 | 0.48 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 11 | 0.48 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 1 | 0.48 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 1 | 0.48 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 1 | 0.48 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 1 | 0.48 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 1 | 0.48 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 1 | 0.48 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 3 | 0.48 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 3 | 0.48 |
| (1,1265) | 1:124:A:GLU:HB3 | 1:125:A:VAL:H | 9 | 0.48 |
| (1,1199) | 1:80:A:ILE:HG21 | 1:105:A:ALA:H | 19 | 0.48 |
| (1,1199) | 1:80:A:ILE:HG22 | 1:105:A:ALA:H | 19 | 0.48 |
| (1,1199) | 1:80:A:ILE:HG23 | 1:105:A:ALA:H | 19 | 0.48 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 1 | 0.48 |
| (1,1049) | 1:81:A:LYS:HD3 | 1:84:A:ASP:H | 8 | 0.48 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 14 | 0.48 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 14 | 0.48 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 14 | 0.48 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 7 | 0.48 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 7 | 0.48 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 7 | 0.48 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 12 | 0.48 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 9 | 0.48 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 12 | 0.48 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 6 | 0.48 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 8 | 0.48 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 20 | 0.48 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 20 | 0.48 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 20 | 0.48 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 19 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 11 | 0.48 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 11 | 0.48 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 11 | 0.48 |
| (1,651) | 1:92:A:LEU:HD11 | 1:129:A:ALA:HA | 4 | 0.48 |
| (1,651) | 1:92:A:LEU:HD12 | 1:129:A:ALA:HA | 4 | 0.48 |
| (1,651) | 1:92:A:LEU:HD13 | 1:129:A:ALA:HA | 4 | 0.48 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 6 | 0.48 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 6 | 0.48 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 6 | 0.48 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 7 | 0.48 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 7 | 0.48 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 7 | 0.48 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 13 | 0.48 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 13 | 0.48 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 13 | 0.48 |
| (1,556) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA3 | 11 | 0.48 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 5 | 0.48 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 13 | 0.48 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 14 | 0.48 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 14 | 0.48 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 10 | 0.48 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 17 | 0.48 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 10 | 0.48 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 10 | 0.48 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 10 | 0.48 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 15 | 0.48 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 15 | 0.48 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 15 | 0.48 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 17 | 0.48 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 17 | 0.48 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 17 | 0.48 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 4 | 0.48 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 15 | 0.48 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 16 | 0.48 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 10 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 10 | 0.48 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 10 | 0.48 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 9 | 0.48 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 10 | 0.48 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 10 | 0.48 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 10 | 0.48 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 12 | 0.48 |
| (1,155) | 1:51:A:ASP:HB3 | 1:124:A:GLU:H | 15 | 0.48 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 11 | 0.48 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 12 | 0.48 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 5 | 0.48 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 5 | 0.48 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 5 | 0.48 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 14 | 0.48 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 14 | 0.48 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 14 | 0.48 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 19 | 0.48 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 19 | 0.48 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 19 | 0.48 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG21 | 18 | 0.48 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG22 | 18 | 0.48 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG23 | 18 | 0.48 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 4 | 0.48 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 11 | 0.48 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 2 | 0.47 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 2 | 0.47 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 9 | 0.47 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 9 | 0.47 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 9 | 0.47 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 9 | 0.47 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 9 | 0.47 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 9 | 0.47 |
| (1,1580) | 1:95:A:LYS:HB2 | 1:128:A:LEU:HD11 | 9 | 0.47 |
| (1,1580) | 1:95:A:LYS:HB2 | 1:128:A:LEU:HD12 | 9 | 0.47 |
| (1,1580) | 1:95:A:LYS:HB2 | 1:128:A:LEU:HD13 | 9 | 0.47 |
| (1,1580) | 1:95:A:LYS:HB2 | 1:128:A:LEU:HD21 | 9 | 0.47 |
| (1,1580) | 1:95:A:LYS:HB2 | 1:128:A:LEU:HD22 | 9 | 0.47 |
| (1,1580) | 1:95:A:LYS:HB2 | 1:128:A:LEU:HD23 | 9 | 0.47 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 2 | 0.47 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 2 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG11 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG12 | 6 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG13 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG21 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG22 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG23 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG11 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG12 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG13 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG21 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG22 | 6 | 0.47 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG23 | 6 | 0.47 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 5 | 0.47 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 5 | 0.47 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 18 | 0.47 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 18 | 0.47 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG2 | 14 | 0.47 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG3 | 14 | 0.47 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG2 | 14 | 0.47 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG3 | 14 | 0.47 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG2 | 14 | 0.47 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG3 | 14 | 0.47 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 7 | 0.47 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 7 | 0.47 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 7 | 0.47 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 11 | 0.47 |
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 11 | 0.47 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 11 | 0.47 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 3 | 0.47 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 3 | 0.47 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 3 | 0.47 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 2 | 0.47 |
| (1,1199) | 1:80:A:ILE:HG21 | 1:105:A:ALA:H | 13 | 0.47 |
| (1,1199) | 1:80:A:ILE:HG22 | 1:105:A:ALA:H | 13 | 0.47 |
| (1,1199) | 1:80:A:ILE:HG23 | 1:105:A:ALA:H | 13 | 0.47 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 4 | 0.47 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 4 | 0.47 |
| (1,1137) | 1:95:A:LYS:HG2 | 1:96:A:ALA:H | 1 | 0.47 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 13 | 0.47 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 5 | 0.47 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 9 | 0.47 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 9 | 0.47 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 9 | 0.47 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 2 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 19 | 0.47 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 13 | 0.47 |
| (1,758) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 3 | 0.47 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 15 | 0.47 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 7 | 0.47 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 5 | 0.47 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 5 | 0.47 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 5 | 0.47 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 1 | 0.47 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 1 | 0.47 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 1 | 0.47 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 15 | 0.47 |
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 3 | 0.47 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 12 | 0.47 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 3 | 0.47 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 4 | 0.47 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 13 | 0.47 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 12 | 0.47 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 15 | 0.47 |
| (1,266) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 14 | 0.47 |
| (1,266) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 14 | 0.47 |
| (1,266) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 14 | 0.47 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 2 | 0.47 |
| (1,228) | 1:47:A:THR:HG21 | 1:69:A:PRO:HA | 16 | 0.47 |
| (1,228) | 1:47:A:THR:HG22 | 1:69:A:PRO:HA | 16 | 0.47 |
| (1,228) | 1:47:A:THR:HG23 | 1:69:A:PRO:HA | 16 | 0.47 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 4 | 0.47 |
| (1,145) | 1:49:A:HIS:HB2 | 1:126:A:GLU:HG2 | 10 | 0.47 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 6 | 0.47 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 6 | 0.47 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 6 | 0.47 |
| (1,38) | 1:31:A:LEU:HG | 1:32:A:THR:H | 3 | 0.47 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 1 | 0.46 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 1 | 0.46 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 1 | 0.46 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 1 | 0.46 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 1 | 0.46 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 1 | 0.46 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 15 | 0.46 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 15 | 0.46 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 2 | 0.46 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 2 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 9 | 0.46 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 9 | 0.46 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 9 | 0.46 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 9 | 0.46 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 9 | 0.46 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 9 | 0.46 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 4 | 0.46 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 4 | 0.46 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD11 | 19 | 0.46 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD12 | 19 | 0.46 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD13 | 19 | 0.46 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD21 | 19 | 0.46 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD22 | 19 | 0.46 |
| (1,1343) | 1:28:A:LYS:HB2 | 1:97:A:LEU:HD23 | 19 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 4 | 0.46 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 4 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1265) | 1:124:A:GLU:HB3 | 1:125:A:VAL:H | 19 | 0.46 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 9 | 0.46 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 9 | 0.46 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 9 | 0.46 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 13 | 0.46 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 13 | 0.46 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 13 | 0.46 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 1 | 0.46 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 5 | 0.46 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 11 | 0.46 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 3 | 0.46 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 6 | 0.46 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 20 | 0.46 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 15 | 0.46 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 3 | 0.46 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 17 | 0.46 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 17 | 0.46 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 17 | 0.46 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 1 | 0.46 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 1 | 0.46 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 1 | 0.46 |
| (1,645) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HG | 2 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 7 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 7 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 7 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 9 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 9 | 0.46 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 9 | 0.46 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 11 | 0.46 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 11 | 0.46 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 11 | 0.46 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 13 | 0.46 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 20 | 0.46 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 20 | 0.46 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 20 | 0.46 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 16 | 0.46 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 16 | 0.46 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 16 | 0.46 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 9 | 0.46 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG21 | 16 | 0.46 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG22 | 16 | 0.46 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG23 | 16 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG21 | 16 | 0.46 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG22 | 16 | 0.46 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG23 | 16 | 0.46 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG21 | 16 | 0.46 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG22 | 16 | 0.46 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG23 | 16 | 0.46 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 13 | 0.46 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 13 | 0.46 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 13 | 0.46 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 20 | 0.46 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG21 | 20 | 0.46 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG22 | 20 | 0.46 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG23 | 20 | 0.46 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 16 | 0.46 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 14 | 0.46 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 14 | 0.46 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 14 | 0.46 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 4 | 0.46 |
| (1,80) | 1:38:A:THR:HB | 1:40:A:PRO:HD2 | 11 | 0.46 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 17 | 0.46 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 17 | 0.46 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 17 | 0.46 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 14 | 0.45 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 14 | 0.45 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 4 | 0.45 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 4 | 0.45 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 4 | 0.45 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 4 | 0.45 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 4 | 0.45 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 4 | 0.45 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 12 | 0.45 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 12 | 0.45 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 12 | 0.45 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 12 | 0.45 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 12 | 0.45 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 12 | 0.45 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 4 | 0.45 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 4 | 0.45 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 15 | 0.45 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 15 | 0.45 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 16 | 0.45 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 16 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 20 | 0.45 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 20 | 0.45 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 19 | 0.45 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 19 | 0.45 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 8 | 0.45 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 8 | 0.45 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 8 | 0.45 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 8 | 0.45 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 7 | 0.45 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 7 | 0.45 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG2 | 19 | 0.45 |
| (1,1333) | 1:24:A:ALA:HB1 | 1:103:A:GLN:HG3 | 19 | 0.45 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG2 | 19 | 0.45 |
| (1,1333) | 1:24:A:ALA:HB2 | 1:103:A:GLN:HG3 | 19 | 0.45 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG2 | 19 | 0.45 |
| (1,1333) | 1:24:A:ALA:HB3 | 1:103:A:GLN:HG3 | 19 | 0.45 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 13 | 0.45 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 13 | 0.45 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 10 | 0.45 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 10 | 0.45 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 18 | 0.45 |
| (1,1276) | 1:96:A:ALA:H | 1:127:A:LEU:H | 18 | 0.45 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 4 | 0.45 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 10 | 0.45 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 2 | 0.45 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 2 | 0.45 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 2 | 0.45 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 2 | 0.45 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 11 | 0.45 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 6 | 0.45 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 6 | 0.45 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 6 | 0.45 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 17 | 0.45 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 17 | 0.45 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 17 | 0.45 |
| (1,950) | 1:64:A:ARG:HA | 1:67:A:GLY:H | 5 | 0.45 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 19 | 0.45 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 4 | 0.45 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 19 | 0.45 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 13 | 0.45 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 17 | 0.45 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 17 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 17 | 0.45 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 10 | 0.45 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 1 | 0.45 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 1 | 0.45 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 1 | 0.45 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG11 | 17 | 0.45 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG12 | 17 | 0.45 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG13 | 17 | 0.45 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 20 | 0.45 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 2 | 0.45 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 2 | 0.45 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 2 | 0.45 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 11 | 0.45 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 19 | 0.45 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 6 | 0.45 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 6 | 0.45 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 6 | 0.45 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 13 | 0.45 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 13 | 0.45 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 13 | 0.45 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG21 | 9 | 0.45 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG22 | 9 | 0.45 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG23 | 9 | 0.45 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 19 | 0.45 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 15 | 0.45 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 15 | 0.45 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 15 | 0.45 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 7 | 0.45 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 8 | 0.45 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 1 | 0.45 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 1 | 0.45 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 1 | 0.45 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 16 | 0.45 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 16 | 0.45 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 1 | 0.45 |
| (1,161) | 1:53:A:ARG:HA | 1:60:A:PHE:H | 13 | 0.45 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 19 | 0.45 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 17 | 0.45 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 19 | 0.45 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 9 | 0.45 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 10 | 0.45 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 10 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 10 | 0.45 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 5 | 0.45 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 5 | 0.45 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 5 | 0.45 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 8 | 0.45 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 8 | 0.45 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 8 | 0.45 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 4 | 0.45 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 4 | 0.45 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 4 | 0.45 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 2 | 0.45 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 18 | 0.44 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 18 | 0.44 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 18 | 0.44 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 18 | 0.44 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 18 | 0.44 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 18 | 0.44 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 12 | 0.44 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 12 | 0.44 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 17 | 0.44 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 17 | 0.44 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 18 | 0.44 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 18 | 0.44 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 19 | 0.44 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 19 | 0.44 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 2 | 0.44 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 2 | 0.44 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 20 | 0.44 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 20 | 0.44 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 10 | 0.44 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 10 | 0.44 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 10 | 0.44 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 10 | 0.44 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 10 | 0.44 |
| (1,1379) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 10 | 0.44 |
| (1,1314) | 1:13:A:GLU:H | 1:13:A:GLU:HB2 | 2 | 0.44 |
| (1,1314) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 2 | 0.44 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 1 | 0.44 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 1 | 0.44 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 1 | 0.44 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 14 | 0.44 |
| (1,1199) | 1:80:A:ILE:HG21 | 1:105:A:ALA:H | 2 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1199) | 1:80:A:ILE:HG22 | 1:105:A:ALA:H | 2 | 0.44 |
| (1,1199) | 1:80:A:ILE:HG23 | 1:105:A:ALA:H | 2 | 0.44 |
| (1,1199) | 1:80:A:ILE:HG21 | 1:105:A:ALA:H | 16 | 0.44 |
| (1,1199) | 1:80:A:ILE:HG22 | 1:105:A:ALA:H | 16 | 0.44 |
| (1,1199) | 1:80:A:ILE:HG23 | 1:105:A:ALA:H | 16 | 0.44 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 14 | 0.44 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 20 | 0.44 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 8 | 0.44 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 5 | 0.44 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 5 | 0.44 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 5 | 0.44 |
| (1,972) | 1:70:A:PHE:HD2 | 1:71:A:GLN:H | 20 | 0.44 |
| (1,952) | 1:67:A:GLY:H | 1:68:A:LYS:HB2 | 5 | 0.44 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 2 | 0.44 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 19 | 0.44 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 7 | 0.44 |
| (1,811) | 1:43:A:GLY:H | 1:74:A:LEU:HB2 | 11 | 0.44 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 19 | 0.44 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 1 | 0.44 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 1 | 0.44 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 1 | 0.44 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 5 | 0.44 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 5 | 0.44 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 5 | 0.44 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 10 | 0.44 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 10 | 0.44 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 10 | 0.44 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 3 | 0.44 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 3 | 0.44 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 3 | 0.44 |
| (1,575) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HG2 | 18 | 0.44 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 2 | 0.44 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 2 | 0.44 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 2 | 0.44 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 17 | 0.44 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 17 | 0.44 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 17 | 0.44 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 10 | 0.44 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 10 | 0.44 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 10 | 0.44 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD21 | 3 | 0.44 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD22 | 3 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD23 | 3 | 0.44 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 5 | 0.44 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 5 | 0.44 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 5 | 0.44 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 19 | 0.44 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 19 | 0.44 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 19 | 0.44 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 5 | 0.44 |
| (1,153) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 12 | 0.44 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 3 | 0.44 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 3 | 0.44 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 3 | 0.44 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 10 | 0.44 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 4 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 4 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 4 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 4 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 4 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 4 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 13 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 13 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 13 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 13 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 13 | 0.43 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 13 | 0.43 |
| (1,1624) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 3 | 0.43 |
| (1,1624) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 3 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 2 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 2 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 2 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 2 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB2 | 12 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HB3 | 12 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB2 | 12 | 0.43 |
| (1,1623) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HB3 | 12 | 0.43 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG2 | 11 | 0.43 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG3 | 11 | 0.43 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 20 | 0.43 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 20 | 0.43 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 20 | 0.43 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 20 | 0.43 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 20 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 20 | 0.43 |
| (1,1584) | 1:95:A:LYS:HG2 | 1:124:A:GLU:HB3 | 19 | 0.43 |
| (1,1584) | 1:95:A:LYS:HG3 | 1:124:A:GLU:HB3 | 19 | 0.43 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 10 | 0.43 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 10 | 0.43 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 7 | 0.43 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 7 | 0.43 |
| (1,1470) | 1:59:A:GLN:H | 1:59:A:GLN:HG2 | 17 | 0.43 |
| (1,1470) | 1:59:A:GLN:H | 1:59:A:GLN:HG3 | 17 | 0.43 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 18 | 0.43 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 18 | 0.43 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 18 | 0.43 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 18 | 0.43 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 18 | 0.43 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 18 | 0.43 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 19 | 0.43 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 19 | 0.43 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 12 | 0.43 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 12 | 0.43 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD11 | 14 | 0.43 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD12 | 14 | 0.43 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD13 | 14 | 0.43 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD21 | 14 | 0.43 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD22 | 14 | 0.43 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD23 | 14 | 0.43 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 1 | 0.43 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 1 | 0.43 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 14 | 0.43 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 4 | 0.43 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 4 | 0.43 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 4 | 0.43 |
| (1,1281) | 1:95:A:LYS:HB2 | 1:127:A:LEU:H | 9 | 0.43 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 3 | 0.43 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 6 | 0.43 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 5 | 0.43 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 5 | 0.43 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 5 | 0.43 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 4 | 0.43 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 4 | 0.43 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 4 | 0.43 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 11 | 0.43 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 18 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 12 | 0.43 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 12 | 0.43 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 12 | 0.43 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 10 | 0.43 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 10 | 0.43 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 10 | 0.43 |
| (1,714) | 1:13:A:GLU:HA | 1:14:A:ALA:H | 2 | 0.43 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 15 | 0.43 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 15 | 0.43 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 15 | 0.43 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 17 | 0.43 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 17 | 0.43 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 17 | 0.43 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 7 | 0.43 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 14 | 0.43 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 6 | 0.43 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 12 | 0.43 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 12 | 0.43 |
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 18 | 0.43 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 18 | 0.43 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 18 | 0.43 |
| (1,232) | 1:48:A:VAL:H | 1:69:A:PRO:HB3 | 4 | 0.43 |
| (1,201) | 1:59:A:GLN:H | 1:59:A:GLN:HG3 | 2 | 0.43 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 17 | 0.43 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 19 | 0.43 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 19 | 0.43 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 19 | 0.43 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 19 | 0.43 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 19 | 0.43 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 19 | 0.43 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 16 | 0.43 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 6 | 0.43 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 4 | 0.43 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 10 | 0.42 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 10 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 10 | 0.42 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 10 | 0.42 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 10 | 0.42 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 10 | 0.42 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 3 | 0.42 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 3 | 0.42 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 6 | 0.42 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 6 | 0.42 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 12 | 0.42 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 12 | 0.42 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 10 | 0.42 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 10 | 0.42 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 13 | 0.42 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 13 | 0.42 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 13 | 0.42 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 13 | 0.42 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 13 | 0.42 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 13 | 0.42 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 1 | 0.42 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 1 | 0.42 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 15 | 0.42 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 15 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 11 | 0.42 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 11 | 0.42 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 20 | 0.42 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 20 | 0.42 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 9 | 0.42 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 18 | 0.42 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 3 | 0.42 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 12 | 0.42 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 12 | 0.42 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 12 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 3 | 0.42 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 11 | 0.42 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 1 | 0.42 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 2 | 0.42 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 14 | 0.42 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 14 | 0.42 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 14 | 0.42 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 15 | 0.42 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 15 | 0.42 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 15 | 0.42 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 20 | 0.42 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 17 | 0.42 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 16 | 0.42 |
| (1,866) | 1:51:A:ASP:H | 1:124:A:GLU:HB3 | 16 | 0.42 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 5 | 0.42 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 5 | 0.42 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 5 | 0.42 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 5 | 0.42 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 6 | 0.42 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 3 | 0.42 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 12 | 0.42 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 12 | 0.42 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 12 | 0.42 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 17 | 0.42 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 17 | 0.42 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 17 | 0.42 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 20 | 0.42 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 20 | 0.42 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 20 | 0.42 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD21 | 2 | 0.42 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD22 | 2 | 0.42 |
| (1,510) | 1:81:A:LYS:HE3 | 1:104:A:LEU:HD23 | 2 | 0.42 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG11 | 17 | 0.42 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG12 | 17 | 0.42 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG13 | 17 | 0.42 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 10 | 0.42 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 19 | 0.42 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 19 | 0.42 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 19 | 0.42 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 19 | 0.42 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 9 | 0.42 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 8 | 0.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 4 | 0.42 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 17 | 0.42 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 15 | 0.42 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 13 | 0.42 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 7 | 0.42 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 7 | 0.42 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 7 | 0.42 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 1 | 0.42 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 1 | 0.42 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 1 | 0.42 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 5 | 0.42 |
| (1,92) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 13 | 0.42 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 19 | 0.42 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG21 | 12 | 0.42 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG22 | 12 | 0.42 |
| (1,60) | 1:38:A:THR:HA | 1:130:A:VAL:HG23 | 12 | 0.42 |
| (1,40) | 1:32:A:THR:HB | 1:95:A:LYS:HB3 | 1 | 0.42 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 14 | 0.42 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 5 | 0.42 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 3 | 0.41 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 3 | 0.41 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 3 | 0.41 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 3 | 0.41 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 3 | 0.41 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 3 | 0.41 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 14 | 0.41 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 14 | 0.41 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 14 | 0.41 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 14 | 0.41 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 14 | 0.41 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 14 | 0.41 |
| (1,1539) | 1:85:A:GLN:HA | 1:85:A:GLN:HE21 | 16 | 0.41 |
| (1,1539) | 1:85:A:GLN:HA | 1:85:A:GLN:HE22 | 16 | 0.41 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 10 | 0.41 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 10 | 0.41 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG11 | 19 | 0.41 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG12 | 19 | 0.41 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG13 | 19 | 0.41 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG21 | 19 | 0.41 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG22 | 19 | 0.41 |
| (1,1480) | 1:60:A:PHE:HD2 | 1:114:A:VAL:HG23 | 19 | 0.41 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 11 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 11 | 0.41 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 8 | 0.41 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 8 | 0.41 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 5 | 0.41 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 5 | 0.41 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG11 | 15 | 0.41 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG12 | 15 | 0.41 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG13 | 15 | 0.41 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG21 | 15 | 0.41 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG22 | 15 | 0.41 |
| (1,1387) | 1:41:A:GLN:H | 1:130:A:VAL:HG23 | 15 | 0.41 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD11 | 4 | 0.41 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD12 | 4 | 0.41 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD13 | 4 | 0.41 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD21 | 4 | 0.41 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD22 | 4 | 0.41 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD23 | 4 | 0.41 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 16 | 0.41 |
| (1,1162) | 1:27:A:GLU:HB2 | 1:99:A:THR:H | 4 | 0.41 |
| (1,1120) | 1:34:A:GLY:HA2 | 1:94:A:GLU:H | 15 | 0.41 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 13 | 0.41 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 13 | 0.41 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 13 | 0.41 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 6 | 0.41 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 6 | 0.41 |
| (1,896) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 9 | 0.41 |
| (1,824) | 1:44:A:LYS:HB3 | 1:45:A:LYS:H | 17 | 0.41 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 6 | 0.41 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 6 | 0.41 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 6 | 0.41 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 15 | 0.41 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 15 | 0.41 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 15 | 0.41 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 7 | 0.41 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 15 | 0.41 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 18 | 0.41 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 8 | 0.41 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 14 | 0.41 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 14 | 0.41 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 14 | 0.41 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 12 | 0.41 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 3 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 17 | 0.41 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 1 | 0.41 |
| (1,522) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HA | 16 | 0.41 |
| (1,522) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HA | 16 | 0.41 |
| (1,522) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HA | 16 | 0.41 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 11 | 0.41 |
| (1,482) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HB2 | 20 | 0.41 |
| (1,482) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HB2 | 20 | 0.41 |
| (1,482) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HB2 | 20 | 0.41 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 15 | 0.41 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 15 | 0.41 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 15 | 0.41 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 4 | 0.41 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 4 | 0.41 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 4 | 0.41 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 2 | 0.41 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 2 | 0.41 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 2 | 0.41 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD11 | 19 | 0.41 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD12 | 19 | 0.41 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD13 | 19 | 0.41 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 18 | 0.41 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 8 | 0.41 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 8 | 0.41 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 8 | 0.41 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 4 | 0.41 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 4 | 0.41 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 4 | 0.41 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 4 | 0.41 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 16 | 0.41 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 16 | 0.41 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 16 | 0.41 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 12 | 0.41 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 1 | 0.41 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 17 | 0.41 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 17 | 0.41 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 17 | 0.41 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 19 | 0.41 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 19 | 0.41 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 19 | 0.41 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 8 | 0.41 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 8 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 8 | 0.41 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 12 | 0.41 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 12 | 0.41 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 12 | 0.41 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 18 | 0.41 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 9 | 0.41 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 9 | 0.41 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 9 | 0.41 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 3 | 0.41 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 3 | 0.41 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 3 | 0.41 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 20 | 0.41 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 18 | 0.41 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG2 | 7 | 0.4 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG3 | 7 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 16 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 16 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 16 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 16 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 16 | 0.4 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 16 | 0.4 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 3 | 0.4 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 3 | 0.4 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 3 | 0.4 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 3 | 0.4 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 11 | 0.4 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 11 | 0.4 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 20 | 0.4 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 20 | 0.4 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 8 | 0.4 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 8 | 0.4 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 8 | 0.4 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 8 | 0.4 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 13 | 0.4 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 13 | 0.4 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 2 | 0.4 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 4 | 0.4 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 19 | 0.4 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 9 | 0.4 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 17 | 0.4 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 6 | 0.4 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 6 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 6 | 0.4 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 5 | 0.4 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 20 | 0.4 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 20 | 0.4 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 20 | 0.4 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 19 | 0.4 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 19 | 0.4 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 19 | 0.4 |
| (1,1029) | 1:82:A:GLY:H | 1:104:A:LEU:HB3 | 19 | 0.4 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 2 | 0.4 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 10 | 0.4 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 10 | 0.4 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 10 | 0.4 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 18 | 0.4 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 10 | 0.4 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 14 | 0.4 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 19 | 0.4 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 4 | 0.4 |
| (1,749) | 1:27:A:GLU:H | 1:27:A:GLU:HG3 | 3 | 0.4 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 15 | 0.4 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 15 | 0.4 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 15 | 0.4 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 20 | 0.4 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 20 | 0.4 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 20 | 0.4 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 18 | 0.4 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 6 | 0.4 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 11 | 0.4 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 15 | 0.4 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 20 | 0.4 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 20 | 0.4 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 20 | 0.4 |
| (1,481) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HA | 20 | 0.4 |
| (1,481) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HA | 20 | 0.4 |
| (1,481) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HA | 20 | 0.4 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 20 | 0.4 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 20 | 0.4 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 20 | 0.4 |
| (1,403) | 1:89:A:THR:HG21 | 1:98:A:PHE:HD2 | 15 | 0.4 |
| (1,403) | 1:89:A:THR:HG22 | 1:98:A:PHE:HD2 | 15 | 0.4 |
| (1,403) | 1:89:A:THR:HG23 | 1:98:A:PHE:HD2 | 15 | 0.4 |
| (1,371) | 1:81:A:LYS:HD3 | 1:84:A:ASP:HB2 | 19 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,343) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 3 | 0.4 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 11 | 0.4 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 11 | 0.4 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 11 | 0.4 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 17 | 0.4 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 17 | 0.4 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 17 | 0.4 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 5 | 0.4 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG21 | 11 | 0.4 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG22 | 11 | 0.4 |
| (1,173) | 1:55:A:PRO:HA | 1:120:A:THR:HG23 | 11 | 0.4 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 4 | 0.4 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 13 | 0.4 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 13 | 0.4 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 13 | 0.4 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 7 | 0.4 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 7 | 0.4 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 7 | 0.4 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 13 | 0.4 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 13 | 0.4 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 13 | 0.4 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 20 | 0.4 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 12 | 0.39 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 12 | 0.39 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 12 | 0.39 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 12 | 0.39 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 12 | 0.39 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 12 | 0.39 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 20 | 0.39 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 20 | 0.39 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 20 | 0.39 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 20 | 0.39 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 20 | 0.39 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 20 | 0.39 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 12 | 0.39 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 12 | 0.39 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 12 | 0.39 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 12 | 0.39 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 12 | 0.39 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 12 | 0.39 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 5 | 0.39 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 5 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 5 | 0.39 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 5 | 0.39 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 5 | 0.39 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 5 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG11 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG12 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG13 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG21 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG22 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG23 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG11 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG12 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG13 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG21 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG22 | 8 | 0.39 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG23 | 8 | 0.39 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 3 | 0.39 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 3 | 0.39 |
| (1,1397) | 1:43:A:GLY:HA2 | 1:44:A:LYS:HG2 | 19 | 0.39 |
| (1,1397) | 1:43:A:GLY:HA2 | 1:44:A:LYS:HG3 | 19 | 0.39 |
| (1,1397) | 1:43:A:GLY:HA3 | 1:44:A:LYS:HG2 | 19 | 0.39 |
| (1,1397) | 1:43:A:GLY:HA3 | 1:44:A:LYS:HG3 | 19 | 0.39 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 12 | 0.39 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 12 | 0.39 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 12 | 0.39 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 12 | 0.39 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 16 | 0.39 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 16 | 0.39 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 20 | 0.39 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 11 | 0.39 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 20 | 0.39 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 9 | 0.39 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 15 | 0.39 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 15 | 0.39 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 15 | 0.39 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 19 | 0.39 |
| (1,950) | 1:64:A:ARG:HA | 1:67:A:GLY:H | 13 | 0.39 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 13 | 0.39 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 1 | 0.39 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 11 | 0.39 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 16 | 0.39 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 13 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 19 | 0.39 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 6 | 0.39 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 8 | 0.39 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 8 | 0.39 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 8 | 0.39 |
| (1,716) | 1:13:A:GLU:HG3 | 1:14:A:ALA:H | 13 | 0.39 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 20 | 0.39 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 20 | 0.39 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 20 | 0.39 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 19 | 0.39 |
| (1,623) | 1:95:A:LYS:HB2 | 1:126:A:GLU:HA | 7 | 0.39 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 5 | 0.39 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 5 | 0.39 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 5 | 0.39 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 5 | 0.39 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 4 | 0.39 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 7 | 0.39 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 3 | 0.39 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG21 | 5 | 0.39 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG22 | 5 | 0.39 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG23 | 5 | 0.39 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 9 | 0.39 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 1 | 0.39 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 19 | 0.39 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 4 | 0.39 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 16 | 0.39 |
| (1,192) | 1:59:A:GLN:HA | 1:61:A:ASP:H | 20 | 0.39 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 20 | 0.39 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 6 | 0.39 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 12 | 0.39 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 15 | 0.39 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 15 | 0.39 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 15 | 0.39 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 16 | 0.39 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 16 | 0.39 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 16 | 0.39 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 20 | 0.39 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 20 | 0.39 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 20 | 0.39 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 6 | 0.39 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 6 | 0.39 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 6 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 12 | 0.39 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 12 | 0.39 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 12 | 0.39 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 4 | 0.39 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB2 | 9 | 0.38 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB3 | 9 | 0.38 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 13 | 0.38 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 13 | 0.38 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 13 | 0.38 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 13 | 0.38 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 13 | 0.38 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 13 | 0.38 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG2 | 12 | 0.38 |
| (1,1452) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HG3 | 12 | 0.38 |
| (1,1441) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 16 | 0.38 |
| (1,1441) | 1:53:A:ARG:HD3 | 1:57:A:GLY:HA2 | 16 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 12 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 12 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 12 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 12 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 12 | 0.38 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 12 | 0.38 |
| (1,1397) | 1:43:A:GLY:HA2 | 1:44:A:LYS:HG2 | 17 | 0.38 |
| (1,1397) | 1:43:A:GLY:HA2 | 1:44:A:LYS:HG3 | 17 | 0.38 |
| (1,1397) | 1:43:A:GLY:HA3 | 1:44:A:LYS:HG2 | 17 | 0.38 |
| (1,1397) | 1:43:A:GLY:HA3 | 1:44:A:LYS:HG3 | 17 | 0.38 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 19 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 19 | 0.38 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 19 | 0.38 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD11 | 18 | 0.38 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD12 | 18 | 0.38 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD13 | 18 | 0.38 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD21 | 18 | 0.38 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD22 | 18 | 0.38 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD23 | 18 | 0.38 |
| (1,1281) | 1:95:A:LYS:HB2 | 1:127:A:LEU:H | 7 | 0.38 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 5 | 0.38 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 2 | 0.38 |
| (1,1162) | 1:27:A:GLU:HB2 | 1:99:A:THR:H | 19 | 0.38 |
| (1,1130) | 1:90:A:MET:HE1 | 1:95:A:LYS:H | 7 | 0.38 |
| (1,1130) | 1:90:A:MET:HE2 | 1:95:A:LYS:H | 7 | 0.38 |
| (1,1130) | 1:90:A:MET:HE3 | 1:95:A:LYS:H | 7 | 0.38 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 10 | 0.38 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 10 | 0.38 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 10 | 0.38 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 20 | 0.38 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 3 | 0.38 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 3 | 0.38 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 3 | 0.38 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 15 | 0.38 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 15 | 0.38 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 15 | 0.38 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 5 | 0.38 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 8 | 0.38 |
| (1,910) | 1:55:A:PRO:HA | 1:57:A:GLY:H | 18 | 0.38 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 15 | 0.38 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 18 | 0.38 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 18 | 0.38 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 18 | 0.38 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 14 | 0.38 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 7 | 0.38 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 7 | 0.38 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 7 | 0.38 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG21 | 2 | 0.38 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG22 | 2 | 0.38 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG23 | 2 | 0.38 |
| (1,708) | 1:11:A:THR:HA | 1:12:A:LEU:H | 17 | 0.38 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 1 | 0.38 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 7 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 10 | 0.38 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 15 | 0.38 |
| (1,528) | 1:80:A:ILE:HG21 | 1:106:A:TYR:HA | 16 | 0.38 |
| (1,528) | 1:80:A:ILE:HG22 | 1:106:A:TYR:HA | 16 | 0.38 |
| (1,528) | 1:80:A:ILE:HG23 | 1:106:A:TYR:HA | 16 | 0.38 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 2 | 0.38 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 6 | 0.38 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 6 | 0.38 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 6 | 0.38 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 4 | 0.38 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 5 | 0.38 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 5 | 0.38 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 5 | 0.38 |
| (1,343) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 11 | 0.38 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 14 | 0.38 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 14 | 0.38 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 14 | 0.38 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 14 | 0.38 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 16 | 0.38 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 19 | 0.38 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 12 | 0.38 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 15 | 0.38 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 9 | 0.38 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 9 | 0.38 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 9 | 0.38 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD21 | 17 | 0.38 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD22 | 17 | 0.38 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD23 | 17 | 0.38 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 8 | 0.38 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 8 | 0.38 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 8 | 0.38 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 3 | 0.38 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 9 | 0.38 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 9 | 0.38 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 9 | 0.38 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 16 | 0.38 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 16 | 0.38 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 16 | 0.38 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 10 | 0.38 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 10 | 0.38 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 10 | 0.38 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 18 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 18 | 0.37 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 18 | 0.37 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 16 | 0.37 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 16 | 0.37 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 1 | 0.37 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 1 | 0.37 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 1 | 0.37 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 1 | 0.37 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 1 | 0.37 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 1 | 0.37 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 16 | 0.37 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 16 | 0.37 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 11 | 0.37 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 19 | 0.37 |
| (1,1265) | 1:124:A:GLU:HB3 | 1:125:A:VAL:H | 8 | 0.37 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 8 | 0.37 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 16 | 0.37 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 7 | 0.37 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 7 | 0.37 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 7 | 0.37 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 7 | 0.37 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 1 | 0.37 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 1 | 0.37 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 1 | 0.37 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 16 | 0.37 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 16 | 0.37 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 16 | 0.37 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 16 | 0.37 |
| (1,1035) | 1:80:A:ILE:HB | 1:83:A:TRP:H | 9 | 0.37 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 7 | 0.37 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 9 | 0.37 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 9 | 0.37 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 9 | 0.37 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 2 | 0.37 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 14 | 0.37 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 13 | 0.37 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 15 | 0.37 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 15 | 0.37 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 1 | 0.37 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 11 | 0.37 |
| (1,813) | 1:43:A:GLY:H | 1:74:A:LEU:HG | 16 | 0.37 |
| (1,797) | 1:41:A:GLN:H | 1:41:A:GLN:HG2 | 19 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 16 | 0.37 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 16 | 0.37 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 16 | 0.37 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 20 | 0.37 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 19 | 0.37 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 5 | 0.37 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 6 | 0.37 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD21 | 20 | 0.37 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD22 | 20 | 0.37 |
| (1,512) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD23 | 20 | 0.37 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 17 | 0.37 |
| (1,417) | 1:90:A:MET:HE1 | 1:94:A:GLU:HG2 | 10 | 0.37 |
| (1,417) | 1:90:A:MET:HE2 | 1:94:A:GLU:HG2 | 10 | 0.37 |
| (1,417) | 1:90:A:MET:HE3 | 1:94:A:GLU:HG2 | 10 | 0.37 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 15 | 0.37 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 15 | 0.37 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 15 | 0.37 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 11 | 0.37 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 11 | 0.37 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 1 | 0.37 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 1 | 0.37 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 1 | 0.37 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 9 | 0.37 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 9 | 0.37 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 9 | 0.37 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 18 | 0.37 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 3 | 0.37 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 10 | 0.37 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 10 | 0.37 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 15 | 0.37 |
| (1,155) | 1:51:A:ASP:HB3 | 1:124:A:GLU:H | 4 | 0.37 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 9 | 0.37 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 5 | 0.37 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 11 | 0.37 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 11 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 1 | 0.37 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 17 | 0.37 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 2 | 0.37 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 4 | 0.36 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 4 | 0.36 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 4 | 0.36 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 4 | 0.36 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 4 | 0.36 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 4 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 12 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 12 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 12 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 12 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 12 | 0.36 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 12 | 0.36 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 8 | 0.36 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 8 | 0.36 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 10 | 0.36 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 10 | 0.36 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 10 | 0.36 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 10 | 0.36 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 10 | 0.36 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 10 | 0.36 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 16 | 0.36 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 16 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 2 | 0.36 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 2 | 0.36 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 10 | 0.36 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 10 | 0.36 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 7 | 0.36 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 16 | 0.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 10 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 10 | 0.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 10 | 0.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 18 | 0.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 18 | 0.36 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 18 | 0.36 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 1 | 0.36 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 7 | 0.36 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 14 | 0.36 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 15 | 0.36 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 9 | 0.36 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 9 | 0.36 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 9 | 0.36 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 6 | 0.36 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 6 | 0.36 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 6 | 0.36 |
| (1,1004) | 1:73:A:THR:HG21 | 1:76:A:ALA:H | 11 | 0.36 |
| (1,1004) | 1:73:A:THR:HG22 | 1:76:A:ALA:H | 11 | 0.36 |
| (1,1004) | 1:73:A:THR:HG23 | 1:76:A:ALA:H | 11 | 0.36 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 2 | 0.36 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 2 | 0.36 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 2 | 0.36 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 12 | 0.36 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 12 | 0.36 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 20 | 0.36 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 10 | 0.36 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 2 | 0.36 |
| (1,685) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG2 | 6 | 0.36 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 6 | 0.36 |
| (1,608) | 1:97:A:LEU:HG | 1:124:A:GLU:HG3 | 14 | 0.36 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 1 | 0.36 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 11 | 0.36 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 12 | 0.36 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 13 | 0.36 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 17 | 0.36 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 18 | 0.36 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 18 | 0.36 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 18 | 0.36 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 18 | 0.36 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 1 | 0.36 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 11 | 0.36 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 11 | 0.36 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 11 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 11 | 0.36 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 17 | 0.36 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 17 | 0.36 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 17 | 0.36 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 4 | 0.36 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 16 | 0.36 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 10 | 0.36 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 6 | 0.36 |
| (1,239) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HG2 | 13 | 0.36 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 15 | 0.36 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 15 | 0.36 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 15 | 0.36 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 15 | 0.36 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 5 | 0.36 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 5 | 0.36 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 5 | 0.36 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 16 | 0.36 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 16 | 0.36 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 16 | 0.36 |
| (1,25) | 1:27:A:GLU:HG3 | 1:28:A:LYS:H | 15 | 0.36 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 3 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 3 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 3 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 3 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 3 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 3 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 9 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 9 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 9 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 9 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 9 | 0.35 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 9 | 0.35 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 5 | 0.35 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 5 | 0.35 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 5 | 0.35 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 5 | 0.35 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 5 | 0.35 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 5 | 0.35 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 14 | 0.35 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 14 | 0.35 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 14 | 0.35 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 14 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 14 | 0.35 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 14 | 0.35 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 10 | 0.35 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 10 | 0.35 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB2 | 16 | 0.35 |
| (1,1451) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HB3 | 16 | 0.35 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 7 | 0.35 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 7 | 0.35 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 20 | 0.35 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 20 | 0.35 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 9 | 0.35 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 9 | 0.35 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 9 | 0.35 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 9 | 0.35 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 4 | 0.35 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 4 | 0.35 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 4 | 0.35 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 18 | 0.35 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 20 | 0.35 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 11 | 0.35 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 7 | 0.35 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 7 | 0.35 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 7 | 0.35 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 6 | 0.35 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 20 | 0.35 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 15 | 0.35 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 15 | 0.35 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 15 | 0.35 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 8 | 0.35 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 8 | 0.35 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 8 | 0.35 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 16 | 0.35 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 16 | 0.35 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 16 | 0.35 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 11 | 0.35 |
| (1,952) | 1:67:A:GLY:H | 1:68:A:LYS:HB2 | 11 | 0.35 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 9 | 0.35 |
| (1,862) | 1:50:A:TYR:HB3 | 1:51:A:ASP:H | 9 | 0.35 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 6 | 0.35 |
| (1,857) | 1:49:A:HIS:HD2 | 1:51:A:ASP:H | 9 | 0.35 |
| (1,824) | 1:44:A:LYS:HB3 | 1:45:A:LYS:H | 16 | 0.35 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG21 | 7 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG22 | 7 | 0.35 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG23 | 7 | 0.35 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 4 | 0.35 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG11 | 20 | 0.35 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG12 | 20 | 0.35 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG13 | 20 | 0.35 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD11 | 4 | 0.35 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD12 | 4 | 0.35 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD13 | 4 | 0.35 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 8 | 0.35 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 3 | 0.35 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 14 | 0.35 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 20 | 0.35 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 7 | 0.35 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB1 | 13 | 0.35 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB2 | 13 | 0.35 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB3 | 13 | 0.35 |
| (1,490) | 1:102:A:TYR:HB3 | 1:102:A:TYR:HE1 | 7 | 0.35 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 17 | 0.35 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 17 | 0.35 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 17 | 0.35 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 20 | 0.35 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 20 | 0.35 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 20 | 0.35 |
| (1,386) | 1:86:A:GLY:HA3 | 1:98:A:PHE:HD2 | 17 | 0.35 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 12 | 0.35 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 20 | 0.35 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 20 | 0.35 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 20 | 0.35 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG21 | 4 | 0.35 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG22 | 4 | 0.35 |
| (1,329) | 1:72:A:PHE:HD2 | 1:79:A:VAL:HG23 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 4 | 0.35 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 4 | 0.35 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 5 | 0.35 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 5 | 0.35 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 5 | 0.35 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 19 | 0.35 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 19 | 0.35 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 19 | 0.35 |
| (1,274) | 1:74:A:LEU:HD11 | 1:87:A:VAL:H | 4 | 0.35 |
| (1,274) | 1:74:A:LEU:HD12 | 1:87:A:VAL:H | 4 | 0.35 |
| (1,274) | 1:74:A:LEU:HD13 | 1:87:A:VAL:H | 4 | 0.35 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 4 | 0.35 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 4 | 0.35 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 4 | 0.35 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 6 | 0.35 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 19 | 0.35 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 6 | 0.35 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 9 | 0.35 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 18 | 0.35 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 3 | 0.35 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 17 | 0.35 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 11 | 0.35 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 12 | 0.35 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 12 | 0.35 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 12 | 0.35 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 11 | 0.35 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 11 | 0.35 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 11 | 0.35 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 5 | 0.35 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 20 | 0.35 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 12 | 0.35 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 1 | 0.35 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 1 | 0.35 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 1 | 0.35 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 5 | 0.35 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 5 | 0.35 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 5 | 0.35 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 17 | 0.35 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 17 | 0.35 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 17 | 0.35 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 15 | 0.35 |
| (1,39) | 1:32:A:THR:HB | 1:95:A:LYS:HB2 | 8 | 0.35 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 9 | 0.35 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 10 | 0.34 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 10 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 10 | 0.34 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 10 | 0.34 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 10 | 0.34 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 10 | 0.34 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 17 | 0.34 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 17 | 0.34 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 15 | 0.34 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 15 | 0.34 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 17 | 0.34 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 17 | 0.34 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 16 | 0.34 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 16 | 0.34 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 13 | 0.34 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 13 | 0.34 |
| (1,1205) | 1:106:A:TYR:H | 1:121:A:LEU:HG | 9 | 0.34 |
| (1,1185) | 1:24:A:ALA:HB1 | 1:103:A:GLN:H | 1 | 0.34 |
| (1,1185) | 1:24:A:ALA:HB2 | 1:103:A:GLN:H | 1 | 0.34 |
| (1,1185) | 1:24:A:ALA:HB3 | 1:103:A:GLN:H | 1 | 0.34 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 12 | 0.34 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 12 | 0.34 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 12 | 0.34 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 5 | 0.34 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 5 | 0.34 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 5 | 0.34 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 2 | 0.34 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 9 | 0.34 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 9 | 0.34 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 9 | 0.34 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 20 | 0.34 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 20 | 0.34 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 20 | 0.34 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 5 | 0.34 |
| (1,965) | 1:69:A:PRO:HG3 | 1:70:A:PHE:H | 1 | 0.34 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 4 | 0.34 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 3 | 0.34 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 1 | 0.34 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 1 | 0.34 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 1 | 0.34 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 11 | 0.34 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 16 | 0.34 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 16 | 0.34 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 16 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 1 | 0.34 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG11 | 8 | 0.34 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG12 | 8 | 0.34 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG13 | 8 | 0.34 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD11 | 20 | 0.34 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD12 | 20 | 0.34 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD13 | 20 | 0.34 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 6 | 0.34 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 7 | 0.34 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 9 | 0.34 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 19 | 0.34 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 20 | 0.34 |
| (1,553) | 1:110:A:GLY:HA2 | 1:115:A:ILE:HB | 4 | 0.34 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 18 | 0.34 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 15 | 0.34 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 14 | 0.34 |
| (1,490) | 1:102:A:TYR:HB3 | 1:102:A:TYR:HE1 | 17 | 0.34 |
| (1,490) | 1:102:A:TYR:HB3 | 1:102:A:TYR:HE1 | 18 | 0.34 |
| (1,461) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 17 | 0.34 |
| (1,461) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 17 | 0.34 |
| (1,461) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 17 | 0.34 |
| (1,456) | 1:28:A:LYS:HB2 | 1:96:A:ALA:HB1 | 3 | 0.34 |
| (1,456) | 1:28:A:LYS:HB2 | 1:96:A:ALA:HB2 | 3 | 0.34 |
| (1,456) | 1:28:A:LYS:HB2 | 1:96:A:ALA:HB3 | 3 | 0.34 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB1 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB2 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB3 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB1 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB2 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB3 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB1 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB2 | 1 | 0.34 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB3 | 1 | 0.34 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 5 | 0.34 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 5 | 0.34 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 5 | 0.34 |
| (1,356) | 1:80:A:ILE:HG12 | 1:83:A:TRP:HB2 | 9 | 0.34 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD11 | 8 | 0.34 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD12 | 8 | 0.34 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD13 | 8 | 0.34 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 2 | 0.34 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 13 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 13 | 0.34 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 13 | 0.34 |
| (1,145) | 1:49:A:HIS:HB2 | 1:126:A:GLU:HG2 | 3 | 0.34 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 10 | 0.34 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 10 | 0.34 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 10 | 0.34 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 6 | 0.34 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 6 | 0.34 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 6 | 0.34 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 10 | 0.34 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 14 | 0.34 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 14 | 0.34 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 14 | 0.34 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 14 | 0.34 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 10 | 0.34 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 6 | 0.33 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 6 | 0.33 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 6 | 0.33 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 6 | 0.33 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 6 | 0.33 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 6 | 0.33 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 20 | 0.33 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 20 | 0.33 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 20 | 0.33 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 20 | 0.33 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 20 | 0.33 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 20 | 0.33 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD11 | 9 | 0.33 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD12 | 9 | 0.33 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD13 | 9 | 0.33 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD21 | 9 | 0.33 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD22 | 9 | 0.33 |
| (1,1509) | 1:69:A:PRO:HG3 | 1:128:A:LEU:HD23 | 9 | 0.33 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 19 | 0.33 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 19 | 0.33 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 4 | 0.33 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 4 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 10 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 10 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 10 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 10 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 10 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 10 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 16 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 16 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 16 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 16 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 16 | 0.33 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 16 | 0.33 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 14 | 0.33 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 14 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG11 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG12 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG13 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG21 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG22 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB2 | 1:122:A:VAL:HG23 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG11 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG12 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG13 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG21 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG22 | 1 | 0.33 |
| (1,1340) | 1:25:A:GLN:HB3 | 1:122:A:VAL:HG23 | 1 | 0.33 |
| (1,1310) | 1:81:A:LYS:HE2 | 1:85:A:GLN:HE22 | 13 | 0.33 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 8 | 0.33 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 9 | 0.33 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 9 | 0.33 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 9 | 0.33 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 1 | 0.33 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 1 | 0.33 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 1 | 0.33 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 10 | 0.33 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 16 | 0.33 |
| (1,1211) | 1:106:A:TYR:HB3 | 1:110:A:GLY:H | 10 | 0.33 |
| (1,1204) | 1:100:A:ILE:HG21 | 1:106:A:TYR:H | 2 | 0.33 |
| (1,1204) | 1:100:A:ILE:HG22 | 1:106:A:TYR:H | 2 | 0.33 |
| (1,1204) | 1:100:A:ILE:HG23 | 1:106:A:TYR:H | 2 | 0.33 |
| (1,1096) | 1:91:A:THR:H | 1:94:A:GLU:H | 7 | 0.33 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 13 | 0.33 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 7 | 0.33 |
| (1,1051) | 1:80:A:ILE:HD11 | 1:84:A:ASP:H | 9 | 0.33 |
| (1,1051) | 1:80:A:ILE:HD12 | 1:84:A:ASP:H | 9 | 0.33 |
| (1,1051) | 1:80:A:ILE:HD13 | 1:84:A:ASP:H | 9 | 0.33 |
| (1,1036) | 1:79:A:VAL:HB | 1:83:A:TRP:H | 6 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 13 | 0.33 |
| (1,862) | 1:50:A:TYR:HB3 | 1:51:A:ASP:H | 16 | 0.33 |
| (1,700) | 1:79:A:VAL:HB | 1:83:A:TRP:HE3 | 1 | 0.33 |
| (1,683) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 2 | 0.33 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 2 | 0.33 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 2 | 0.33 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 2 | 0.33 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 19 | 0.33 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 19 | 0.33 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 19 | 0.33 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 20 | 0.33 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG11 | 11 | 0.33 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG12 | 11 | 0.33 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG13 | 11 | 0.33 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 6 | 0.33 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 6 | 0.33 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 6 | 0.33 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 8 | 0.33 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 6 | 0.33 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 18 | 0.33 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 5 | 0.33 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 8 | 0.33 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 8 | 0.33 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 11 | 0.33 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB1 | 14 | 0.33 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB2 | 14 | 0.33 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB3 | 14 | 0.33 |
| (1,490) | 1:102:A:TYR:HB3 | 1:102:A:TYR:HE1 | 4 | 0.33 |
| (1,424) | 1:34:A:GLY:HA3 | 1:91:A:THR:HB | 11 | 0.33 |
| (1,424) | 1:34:A:GLY:HA3 | 1:91:A:THR:HB | 15 | 0.33 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 9 | 0.33 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 9 | 0.33 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 9 | 0.33 |
| (1,389) | 1:87:A:VAL:HA | 1:90:A:MET:HG3 | 6 | 0.33 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 3 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 3 | 0.33 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 3 | 0.33 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 18 | 0.33 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 18 | 0.33 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 18 | 0.33 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 13 | 0.33 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 15 | 0.33 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 1 | 0.33 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 1 | 0.33 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 1 | 0.33 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 6 | 0.33 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 2 | 0.33 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 5 | 0.33 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 8 | 0.33 |
| (1,155) | 1:51:A:ASP:HB3 | 1:124:A:GLU:H | 5 | 0.33 |
| (1,153) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 18 | 0.33 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 15 | 0.33 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 15 | 0.33 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 15 | 0.33 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 11 | 0.33 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 11 | 0.33 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 11 | 0.33 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 20 | 0.33 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 20 | 0.33 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 20 | 0.33 |
| (1,109) | 1:46:A:VAL:HB | 1:129:A:ALA:H | 8 | 0.33 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 17 | 0.33 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 14 | 0.33 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 14 | 0.33 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 14 | 0.33 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 6 | 0.33 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 12 | 0.33 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 10 | 0.33 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 5 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 5 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 5 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 5 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 5 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 5 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 9 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 9 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 9 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 9 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 9 | 0.32 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 9 | 0.32 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 8 | 0.32 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 8 | 0.32 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 8 | 0.32 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 8 | 0.32 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 8 | 0.32 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 8 | 0.32 |
| (1,1575) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 8 | 0.32 |
| (1,1575) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 8 | 0.32 |
| (1,1575) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 8 | 0.32 |
| (1,1575) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 8 | 0.32 |
| (1,1575) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 8 | 0.32 |
| (1,1575) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 8 | 0.32 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 8 | 0.32 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 8 | 0.32 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 6 | 0.32 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 6 | 0.32 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD11 | 10 | 0.32 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD12 | 10 | 0.32 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD13 | 10 | 0.32 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD21 | 10 | 0.32 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD22 | 10 | 0.32 |
| (1,1372) | 1:38:A:THR:HA | 1:92:A:LEU:HD23 | 10 | 0.32 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 7 | 0.32 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 7 | 0.32 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 7 | 0.32 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 5 | 0.32 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 20 | 0.32 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 20 | 0.32 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 20 | 0.32 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 14 | 0.32 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 14 | 0.32 |
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 14 | 0.32 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 13 | 0.32 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 8 | 0.32 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 3 | 0.32 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 3 | 0.32 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 3 | 0.32 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 16 | 0.32 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 16 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 16 | 0.32 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 8 | 0.32 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 8 | 0.32 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 8 | 0.32 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 13 | 0.32 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB1 | 6 | 0.32 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB2 | 6 | 0.32 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB3 | 6 | 0.32 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 17 | 0.32 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 3 | 0.32 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 6 | 0.32 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 6 | 0.32 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 6 | 0.32 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 8 | 0.32 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 3 | 0.32 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 3 | 0.32 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 3 | 0.32 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 10 | 0.32 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 10 | 0.32 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 10 | 0.32 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 10 | 0.32 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 10 | 0.32 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 10 | 0.32 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 16 | 0.32 |
| (1,585) | 1:121:A:LEU:HG | 1:123:A:PHE:HD1 | 8 | 0.32 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 20 | 0.32 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 14 | 0.32 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 14 | 0.32 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 14 | 0.32 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 11 | 0.32 |
| (1,421) | 1:91:A:THR:HA | 1:127:A:LEU:HG | 15 | 0.32 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 16 | 0.32 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 16 | 0.32 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 16 | 0.32 |
| (1,385) | 1:82:A:GLY:HA2 | 1:85:A:GLN:HB3 | 18 | 0.32 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 3 | 0.32 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 8 | 0.32 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 8 | 0.32 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 8 | 0.32 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 8 | 0.32 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 7 | 0.32 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 3 | 0.32 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 1 | 0.32 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 18 | 0.32 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 11 | 0.32 |
| (1,145) | 1:49:A:HIS:HB2 | 1:126:A:GLU:HG2 | 14 | 0.32 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 4 | 0.32 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 4 | 0.32 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 4 | 0.32 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 1 | 0.32 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 2 | 0.32 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 12 | 0.32 |
| (1,92) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG2 | 6 | 0.32 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 6 | 0.32 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 6 | 0.32 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 6 | 0.32 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 3 | 0.32 |
| (1,48) | 1:34:A:GLY:HA2 | 1:94:A:GLU:HB3 | 11 | 0.32 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 6 | 0.32 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 17 | 0.32 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 3 | 0.32 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 6 | 0.32 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG11 | 17 | 0.31 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG12 | 17 | 0.31 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG13 | 17 | 0.31 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG21 | 17 | 0.31 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG22 | 17 | 0.31 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG23 | 17 | 0.31 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 3 | 0.31 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 3 | 0.31 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 3 | 0.31 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 3 | 0.31 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 3 | 0.31 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 3 | 0.31 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 9 | 0.31 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 9 | 0.31 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 12 | 0.31 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 12 | 0.31 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 12 | 0.31 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 12 | 0.31 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 12 | 0.31 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 12 | 0.31 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 9 | 0.31 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 9 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 8 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 8 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 8 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 8 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 8 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 8 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 17 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 17 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 17 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 17 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 17 | 0.31 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 17 | 0.31 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 12 | 0.31 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 12 | 0.31 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 16 | 0.31 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 16 | 0.31 |
| (1,1405) | 1:44:A:LYS:HE2 | 1:45:A:LYS:H | 3 | 0.31 |
| (1,1405) | 1:44:A:LYS:HE3 | 1:45:A:LYS:H | 3 | 0.31 |
| (1,1308) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 16 | 0.31 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 13 | 0.31 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 13 | 0.31 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 13 | 0.31 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 5 | 0.31 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 14 | 0.31 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 17 | 0.31 |
| (1,1197) | 1:100:A:ILE:HG21 | 1:105:A:ALA:H | 7 | 0.31 |
| (1,1197) | 1:100:A:ILE:HG22 | 1:105:A:ALA:H | 7 | 0.31 |
| (1,1197) | 1:100:A:ILE:HG23 | 1:105:A:ALA:H | 7 | 0.31 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 6 | 0.31 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 12 | 0.31 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 19 | 0.31 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 19 | 0.31 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 19 | 0.31 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 1 | 0.31 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 11 | 0.31 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 10 | 0.31 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 3 | 0.31 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 10 | 0.31 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 4 | 0.31 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 10 | 0.31 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 12 | 0.31 |
| (1,819) | 1:44:A:LYS:H | 1:44:A:LYS:HG2 | 17 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 20 | 0.31 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 20 | 0.31 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 20 | 0.31 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 15 | 0.31 |
| (1,749) | 1:27:A:GLU:H | 1:27:A:GLU:HG3 | 1 | 0.31 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 14 | 0.31 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 3 | 0.31 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 3 | 0.31 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 3 | 0.31 |
| (1,681) | 1:50:A:TYR:H | 1:50:A:TYR:HD2 | 9 | 0.31 |
| (1,644) | 1:49:A:HIS:HB2 | 1:128:A:LEU:HG | 13 | 0.31 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 17 | 0.31 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 13 | 0.31 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 9 | 0.31 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB1 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB2 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB3 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB1 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB2 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB3 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB1 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB2 | 8 | 0.31 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB3 | 8 | 0.31 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 9 | 0.31 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 2 | 0.31 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 2 | 0.31 |
| (1,520) | 1:100:A:ILE:HG21 | 1:105:A:ALA:HA | 7 | 0.31 |
| (1,520) | 1:100:A:ILE:HG22 | 1:105:A:ALA:HA | 7 | 0.31 |
| (1,520) | 1:100:A:ILE:HG23 | 1:105:A:ALA:HA | 7 | 0.31 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG21 | 4 | 0.31 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG22 | 4 | 0.31 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG23 | 4 | 0.31 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 13 | 0.31 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 5 | 0.31 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 5 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 5 | 0.31 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD21 | 20 | 0.31 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD22 | 20 | 0.31 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD23 | 20 | 0.31 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 15 | 0.31 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 15 | 0.31 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 15 | 0.31 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 15 | 0.31 |
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 3 | 0.31 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 3 | 0.31 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 3 | 0.31 |
| (1,192) | 1:59:A:GLN:HA | 1:61:A:ASP:H | 16 | 0.31 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 10 | 0.31 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 16 | 0.31 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 16 | 0.31 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 16 | 0.31 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 10 | 0.31 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG21 | 6 | 0.31 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG22 | 6 | 0.31 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG23 | 6 | 0.31 |
| (1,76) | 1:38:A:THR:HB | 1:40:A:PRO:HD3 | 7 | 0.31 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 14 | 0.31 |
| (1,71) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 14 | 0.31 |
| (1,21) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 8 | 0.31 |
| (1,18) | 1:41:A:GLN:HA | 1:74:A:LEU:HD21 | 6 | 0.31 |
| (1,18) | 1:41:A:GLN:HA | 1:74:A:LEU:HD22 | 6 | 0.31 |
| (1,18) | 1:41:A:GLN:HA | 1:74:A:LEU:HD23 | 6 | 0.31 |
| (1,1619) | 1:103:A:GLN:HG2 | 1:104:A:LEU:H | 4 | 0.3 |
| (1,1619) | 1:103:A:GLN:HG3 | 1:104:A:LEU:H | 4 | 0.3 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG2 | 16 | 0.3 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG3 | 16 | 0.3 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 15 | 0.3 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 15 | 0.3 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 15 | 0.3 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 15 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 15 | 0.3 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 15 | 0.3 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 9 | 0.3 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 9 | 0.3 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 9 | 0.3 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 9 | 0.3 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 9 | 0.3 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 9 | 0.3 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 4 | 0.3 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 4 | 0.3 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 12 | 0.3 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 12 | 0.3 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 18 | 0.3 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 18 | 0.3 |
| (1,1475) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 14 | 0.3 |
| (1,1475) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 14 | 0.3 |
| (1,1475) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 18 | 0.3 |
| (1,1475) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 18 | 0.3 |
| (1,1470) | 1:59:A:GLN:H | 1:59:A:GLN:HG2 | 2 | 0.3 |
| (1,1470) | 1:59:A:GLN:H | 1:59:A:GLN:HG3 | 2 | 0.3 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 7 | 0.3 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 7 | 0.3 |
| (1,1441) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 2 | 0.3 |
| (1,1441) | 1:53:A:ARG:HD3 | 1:57:A:GLY:HA2 | 2 | 0.3 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 16 | 0.3 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 16 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 2 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 2 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 2 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 2 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 2 | 0.3 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 2 | 0.3 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 9 | 0.3 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 9 | 0.3 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 18 | 0.3 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 18 | 0.3 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 2 | 0.3 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 2 | 0.3 |
| (1,1405) | 1:44:A:LYS:HE2 | 1:45:A:LYS:H | 9 | 0.3 |
| (1,1405) | 1:44:A:LYS:HE3 | 1:45:A:LYS:H | 9 | 0.3 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 3 | 0.3 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 3 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 3 | 0.3 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 3 | 0.3 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 4 | 0.3 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 4 | 0.3 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 7 | 0.3 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 7 | 0.3 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 5 | 0.3 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 5 | 0.3 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 11 | 0.3 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 11 | 0.3 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 6 | 0.3 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 7 | 0.3 |
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 7 | 0.3 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 7 | 0.3 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 9 | 0.3 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 5 | 0.3 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 5 | 0.3 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 5 | 0.3 |
| (1,1105) | 1:38:A:THR:H | 1:92:A:LEU:H | 2 | 0.3 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 14 | 0.3 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 14 | 0.3 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 14 | 0.3 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 3 | 0.3 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 3 | 0.3 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 3 | 0.3 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB1 | 2 | 0.3 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB2 | 2 | 0.3 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB3 | 2 | 0.3 |
| (1,972) | 1:70:A:PHE:HD2 | 1:71:A:GLN:H | 3 | 0.3 |
| (1,953) | 1:49:A:HIS:HE1 | 1:68:A:LYS:H | 10 | 0.3 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 17 | 0.3 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 14 | 0.3 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 10 | 0.3 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 20 | 0.3 |
| (1,866) | 1:51:A:ASP:H | 1:124:A:GLU:HB3 | 12 | 0.3 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 4 | 0.3 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 8 | 0.3 |
| (1,858) | 1:50:A:TYR:HD1 | 1:51:A:ASP:H | 16 | 0.3 |
| (1,824) | 1:44:A:LYS:HB3 | 1:45:A:LYS:H | 14 | 0.3 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 5 | 0.3 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 6 | 0.3 |
| (1,777) | 1:34:A:GLY:H | 1:91:A:THR:HG21 | 17 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,777) | 1:34:A:GLY:H | 1:91:A:THR:HG22 | 17 | 0.3 |
| (1,777) | 1:34:A:GLY:H | 1:91:A:THR:HG23 | 17 | 0.3 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 8 | 0.3 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 8 | 0.3 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 8 | 0.3 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 5 | 0.3 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 5 | 0.3 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 5 | 0.3 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 13 | 0.3 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 13 | 0.3 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 13 | 0.3 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 15 | 0.3 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 7 | 0.3 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 18 | 0.3 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 18 | 0.3 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 18 | 0.3 |
| (1,593) | 1:122:A:VAL:HA | 1:123:A:PHE:HB3 | 2 | 0.3 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 16 | 0.3 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 16 | 0.3 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 16 | 0.3 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 13 | 0.3 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 3 | 0.3 |
| (1,534) | 1:106:A:TYR:HB2 | 1:111:A:TYR:HD2 | 4 | 0.3 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB1 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB2 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG21 | 1:105:A:ALA:HB3 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB1 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB2 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG22 | 1:105:A:ALA:HB3 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB1 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB2 | 15 | 0.3 |
| (1,525) | 1:80:A:ILE:HG23 | 1:105:A:ALA:HB3 | 15 | 0.3 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 5 | 0.3 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 5 | 0.3 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 5 | 0.3 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 3 | 0.3 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 3 | 0.3 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 3 | 0.3 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 14 | 0.3 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 14 | 0.3 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 14 | 0.3 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 1 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 19 | 0.3 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 19 | 0.3 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 19 | 0.3 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 15 | 0.3 |
| (1,238) | 1:69:A:PRO:HG2 | 1:128:A:LEU:HG | 10 | 0.3 |
| (1,237) | 1:69:A:PRO:HB2 | 1:70:A:PHE:H | 19 | 0.3 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 17 | 0.3 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 16 | 0.3 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 16 | 0.3 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 9 | 0.3 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 12 | 0.3 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 12 | 0.3 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 12 | 0.3 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 15 | 0.3 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 15 | 0.3 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 15 | 0.3 |
| (1,72) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 12 | 0.3 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 20 | 0.3 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 20 | 0.3 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 20 | 0.3 |
| (1,27) | 1:27:A:GLU:HG3 | 1:99:A:THR:HB | 19 | 0.3 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 15 | 0.3 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 20 | 0.29 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 20 | 0.29 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 20 | 0.29 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 20 | 0.29 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 20 | 0.29 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 20 | 0.29 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 19 | 0.29 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 19 | 0.29 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 19 | 0.29 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 19 | 0.29 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 19 | 0.29 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 19 | 0.29 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 2 | 0.29 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 2 | 0.29 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 2 | 0.29 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 2 | 0.29 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 2 | 0.29 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 2 | 0.29 |
| (1,1558) | 1:89:A:THR:H | 1:90:A:MET:HG2 | 6 | 0.29 |
| (1,1558) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 6 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 1 | 0.29 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 1 | 0.29 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 16 | 0.29 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 16 | 0.29 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 16 | 0.29 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 16 | 0.29 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 16 | 0.29 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 16 | 0.29 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 20 | 0.29 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 20 | 0.29 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 20 | 0.29 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 20 | 0.29 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 20 | 0.29 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 20 | 0.29 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 3 | 0.29 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 3 | 0.29 |
| (1,1405) | 1:44:A:LYS:HE2 | 1:45:A:LYS:H | 18 | 0.29 |
| (1,1405) | 1:44:A:LYS:HE3 | 1:45:A:LYS:H | 18 | 0.29 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD2 | 18 | 0.29 |
| (1,1395) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HD3 | 18 | 0.29 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD2 | 18 | 0.29 |
| (1,1395) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HD3 | 18 | 0.29 |
| (1,1382) | 1:40:A:PRO:HB2 | 1:74:A:LEU:HD21 | 7 | 0.29 |
| (1,1382) | 1:40:A:PRO:HB2 | 1:74:A:LEU:HD22 | 7 | 0.29 |
| (1,1382) | 1:40:A:PRO:HB2 | 1:74:A:LEU:HD23 | 7 | 0.29 |
| (1,1382) | 1:40:A:PRO:HB3 | 1:74:A:LEU:HD21 | 7 | 0.29 |
| (1,1382) | 1:40:A:PRO:HB3 | 1:74:A:LEU:HD22 | 7 | 0.29 |
| (1,1382) | 1:40:A:PRO:HB3 | 1:74:A:LEU:HD23 | 7 | 0.29 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 18 | 0.29 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 17 | 0.29 |
| (1,1197) | 1:100:A:ILE:HG21 | 1:105:A:ALA:H | 4 | 0.29 |
| (1,1197) | 1:100:A:ILE:HG22 | 1:105:A:ALA:H | 4 | 0.29 |
| (1,1197) | 1:100:A:ILE:HG23 | 1:105:A:ALA:H | 4 | 0.29 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 16 | 0.29 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 7 | 0.29 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 6 | 0.29 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 16 | 0.29 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 7 | 0.29 |
| (1,1065) | 1:79:A:VAL:HG21 | 1:85:A:GLN:H | 11 | 0.29 |
| (1,1065) | 1:79:A:VAL:HG22 | 1:85:A:GLN:H | 11 | 0.29 |
| (1,1065) | 1:79:A:VAL:HG23 | 1:85:A:GLN:H | 11 | 0.29 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 3 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 3 | 0.29 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 3 | 0.29 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 10 | 0.29 |
| (1,972) | 1:70:A:PHE:HD2 | 1:71:A:GLN:H | 6 | 0.29 |
| (1,972) | 1:70:A:PHE:HD2 | 1:71:A:GLN:H | 16 | 0.29 |
| (1,929) | 1:63:A:SER:H | 1:64:A:ARG:HG3 | 11 | 0.29 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 5 | 0.29 |
| (1,881) | 1:54:A:PHE:H | 1:54:A:PHE:HD1 | 15 | 0.29 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 1 | 0.29 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 7 | 0.29 |
| (1,813) | 1:43:A:GLY:H | 1:74:A:LEU:HG | 18 | 0.29 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 9 | 0.29 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 9 | 0.29 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 9 | 0.29 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 18 | 0.29 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 18 | 0.29 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 18 | 0.29 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 3 | 0.29 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 3 | 0.29 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 3 | 0.29 |
| (1,690) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD2 | 11 | 0.29 |
| (1,681) | 1:50:A:TYR:H | 1:50:A:TYR:HD2 | 3 | 0.29 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 17 | 0.29 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 17 | 0.29 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 17 | 0.29 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 1 | 0.29 |
| (1,611) | 1:123:A:PHE:H | 1:124:A:GLU:HG3 | 6 | 0.29 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 1 | 0.29 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 12 | 0.29 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 12 | 0.29 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 12 | 0.29 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 6 | 0.29 |
| (1,541) | 1:108:A:GLU:HA | 1:118:A:LYS:HA | 15 | 0.29 |
| (1,520) | 1:100:A:ILE:HG21 | 1:105:A:ALA:HA | 4 | 0.29 |
| (1,520) | 1:100:A:ILE:HG22 | 1:105:A:ALA:HA | 4 | 0.29 |
| (1,520) | 1:100:A:ILE:HG23 | 1:105:A:ALA:HA | 4 | 0.29 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD11 | 13 | 0.29 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD12 | 13 | 0.29 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD13 | 13 | 0.29 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG21 | 11 | 0.29 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG22 | 11 | 0.29 |
| (1,469) | 1:27:A:GLU:HB2 | 1:99:A:THR:HG23 | 11 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,430) | 1:92:A:LEU:HD21 | 1:129:A:ALA:HA | 3 | 0.29 |
| (1,430) | 1:92:A:LEU:HD22 | 1:129:A:ALA:HA | 3 | 0.29 |
| (1,430) | 1:92:A:LEU:HD23 | 1:129:A:ALA:HA | 3 | 0.29 |
| (1,417) | 1:90:A:MET:HE1 | 1:94:A:GLU:HG2 | 15 | 0.29 |
| (1,417) | 1:90:A:MET:HE2 | 1:94:A:GLU:HG2 | 15 | 0.29 |
| (1,417) | 1:90:A:MET:HE3 | 1:94:A:GLU:HG2 | 15 | 0.29 |
| (1,395) | 1:40:A:PRO:HG2 | 1:88:A:ALA:HA | 18 | 0.29 |
| (1,336) | 1:81:A:LYS:HB3 | 1:81:A:LYS:HE2 | 19 | 0.29 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 1 | 0.29 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 1 | 0.29 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 1 | 0.29 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 7 | 0.29 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 7 | 0.29 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 7 | 0.29 |
| (1,286) | 1:74:A:LEU:HA | 1:76:A:ALA:HB1 | 14 | 0.29 |
| (1,286) | 1:74:A:LEU:HA | 1:76:A:ALA:HB2 | 14 | 0.29 |
| (1,286) | 1:74:A:LEU:HA | 1:76:A:ALA:HB3 | 14 | 0.29 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 11 | 0.29 |
| (1,227) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 17 | 0.29 |
| (1,220) | 1:66:A:ARG:HA | 1:66:A:ARG:HD2 | 6 | 0.29 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 4 | 0.29 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 15 | 0.29 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 8 | 0.29 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 7 | 0.29 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 7 | 0.29 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 7 | 0.29 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD11 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD12 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD13 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD11 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD12 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD13 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD11 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD12 | 11 | 0.29 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD13 | 11 | 0.29 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 2 | 0.29 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 2 | 0.29 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 2 | 0.29 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 15 | 0.29 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 11 | 0.29 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 11 | 0.29 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 11 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 4 | 0.29 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 4 | 0.29 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 4 | 0.29 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG2 | 18 | 0.28 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG3 | 18 | 0.28 |
| (1,1592) | 1:97:A:LEU:HD11 | 1:98:A:PHE:HD1 | 18 | 0.28 |
| (1,1592) | 1:97:A:LEU:HD12 | 1:98:A:PHE:HD1 | 18 | 0.28 |
| (1,1592) | 1:97:A:LEU:HD13 | 1:98:A:PHE:HD1 | 18 | 0.28 |
| (1,1592) | 1:97:A:LEU:HD21 | 1:98:A:PHE:HD1 | 18 | 0.28 |
| (1,1592) | 1:97:A:LEU:HD22 | 1:98:A:PHE:HD1 | 18 | 0.28 |
| (1,1592) | 1:97:A:LEU:HD23 | 1:98:A:PHE:HD1 | 18 | 0.28 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 19 | 0.28 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 19 | 0.28 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 19 | 0.28 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 19 | 0.28 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 19 | 0.28 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 19 | 0.28 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 14 | 0.28 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 14 | 0.28 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 19 | 0.28 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 19 | 0.28 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 19 | 0.28 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 19 | 0.28 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 19 | 0.28 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 19 | 0.28 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 20 | 0.28 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 20 | 0.28 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 3 | 0.28 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 3 | 0.28 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 3 | 0.28 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 3 | 0.28 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 3 | 0.28 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 3 | 0.28 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 16 | 0.28 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 16 | 0.28 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 12 | 0.28 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 12 | 0.28 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 12 | 0.28 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 12 | 0.28 |
| (1,1323) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HB2 | 11 | 0.28 |
| (1,1323) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HB2 | 11 | 0.28 |
| (1,1314) | 1:13:A:GLU:H | 1:13:A:GLU:HB2 | 19 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1314) | 1:13:A:GLU:H | 1:13:A:GLU:HB3 | 19 | 0.28 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 19 | 0.28 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 19 | 0.28 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 19 | 0.28 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 11 | 0.28 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 11 | 0.28 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 11 | 0.28 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 9 | 0.28 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 13 | 0.28 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 18 | 0.28 |
| (1,1215) | 1:110:A:GLY:HA3 | 1:111:A:TYR:H | 8 | 0.28 |
| (1,1213) | 1:109:A:ARG:HB3 | 1:110:A:GLY:H | 15 | 0.28 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 9 | 0.28 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 9 | 0.28 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 9 | 0.28 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 10 | 0.28 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 10 | 0.28 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 10 | 0.28 |
| (1,1156) | 1:97:A:LEU:HD21 | 1:98:A:PHE:H | 14 | 0.28 |
| (1,1156) | 1:97:A:LEU:HD22 | 1:98:A:PHE:H | 14 | 0.28 |
| (1,1156) | 1:97:A:LEU:HD23 | 1:98:A:PHE:H | 14 | 0.28 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 12 | 0.28 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 12 | 0.28 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 12 | 0.28 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 17 | 0.28 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 17 | 0.28 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 17 | 0.28 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 5 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 15 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 15 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 15 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 17 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 17 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 17 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 18 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 18 | 0.28 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 18 | 0.28 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 15 | 0.28 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 15 | 0.28 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 15 | 0.28 |
| (1,862) | 1:50:A:TYR:HB3 | 1:51:A:ASP:H | 3 | 0.28 |
| (1,858) | 1:50:A:TYR:HD1 | 1:51:A:ASP:H | 5 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 9 | 0.28 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 14 | 0.28 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 15 | 0.28 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 3 | 0.28 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 15 | 0.28 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 18 | 0.28 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 10 | 0.28 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 10 | 0.28 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 10 | 0.28 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 20 | 0.28 |
| (1,545) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 11 | 0.28 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 6 | 0.28 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 14 | 0.28 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 18 | 0.28 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 1 | 0.28 |
| (1,528) | 1:80:A:ILE:HG21 | 1:106:A:TYR:HA | 2 | 0.28 |
| (1,528) | 1:80:A:ILE:HG22 | 1:106:A:TYR:HA | 2 | 0.28 |
| (1,528) | 1:80:A:ILE:HG23 | 1:106:A:TYR:HA | 2 | 0.28 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 13 | 0.28 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB1 | 2 | 0.28 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB2 | 2 | 0.28 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB3 | 2 | 0.28 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG11 | 20 | 0.28 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG12 | 20 | 0.28 |
| (1,465) | 1:99:A:THR:HB | 1:122:A:VAL:HG13 | 20 | 0.28 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 13 | 0.28 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 13 | 0.28 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 13 | 0.28 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 20 | 0.28 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 20 | 0.28 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 20 | 0.28 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 3 | 0.28 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 3 | 0.28 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 3 | 0.28 |
| (1,336) | 1:81:A:LYS:HB3 | 1:81:A:LYS:HE2 | 8 | 0.28 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 12 | 0.28 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 12 | 0.28 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 12 | 0.28 |
| (1,212) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 12 | 0.28 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 5 | 0.28 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 17 | 0.28 |
| (1,192) | 1:59:A:GLN:HA | 1:61:A:ASP:H | 10 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 1 | 0.28 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 8 | 0.28 |
| (1,161) | 1:53:A:ARG:HA | 1:60:A:PHE:H | 4 | 0.28 |
| (1,150) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG11 | 11 | 0.28 |
| (1,150) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG12 | 11 | 0.28 |
| (1,150) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG13 | 11 | 0.28 |
| (1,117) | 1:46:A:VAL:HG21 | 1:48:A:VAL:HA | 8 | 0.28 |
| (1,117) | 1:46:A:VAL:HG22 | 1:48:A:VAL:HA | 8 | 0.28 |
| (1,117) | 1:46:A:VAL:HG23 | 1:48:A:VAL:HA | 8 | 0.28 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 16 | 0.28 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 7 | 0.28 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 7 | 0.28 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 7 | 0.28 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG21 | 15 | 0.28 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG22 | 15 | 0.28 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG23 | 15 | 0.28 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 1 | 0.28 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 1 | 0.28 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 1 | 0.28 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 9 | 0.28 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 9 | 0.28 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 9 | 0.28 |
| (1,48) | 1:34:A:GLY:HA2 | 1:94:A:GLU:HB3 | 16 | 0.28 |
| (1,9) | 1:23:A:SER:HB2 | 1:24:A:ALA:HB1 | 3 | 0.28 |
| (1,9) | 1:23:A:SER:HB2 | 1:24:A:ALA:HB2 | 3 | 0.28 |
| (1,9) | 1:23:A:SER:HB2 | 1:24:A:ALA:HB3 | 3 | 0.28 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 10 | 0.28 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 17 | 0.27 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 17 | 0.27 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 17 | 0.27 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 17 | 0.27 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 17 | 0.27 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 17 | 0.27 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 6 | 0.27 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 6 | 0.27 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 13 | 0.27 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 13 | 0.27 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG21 | 20 | 0.27 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG22 | 20 | 0.27 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG23 | 20 | 0.27 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG21 | 20 | 0.27 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG22 | 20 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG23 | 20 | 0.27 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 13 | 0.27 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 13 | 0.27 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG11 | 18 | 0.27 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG12 | 18 | 0.27 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG13 | 18 | 0.27 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG11 | 18 | 0.27 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG12 | 18 | 0.27 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG13 | 18 | 0.27 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD21 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD22 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD23 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD21 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD22 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD23 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD21 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD22 | 15 | 0.27 |
| (1,1376) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD23 | 15 | 0.27 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 2 | 0.27 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 2 | 0.27 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 2 | 0.27 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 2 | 0.27 |
| (1,1276) | 1:96:A:ALA:H | 1:127:A:LEU:H | 14 | 0.27 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 3 | 0.27 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 8 | 0.27 |
| (1,1245) | 1:120:A:THR:HG21 | 1:122:A:VAL:H | 11 | 0.27 |
| (1,1245) | 1:120:A:THR:HG22 | 1:122:A:VAL:H | 11 | 0.27 |
| (1,1245) | 1:120:A:THR:HG23 | 1:122:A:VAL:H | 11 | 0.27 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 8 | 0.27 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 8 | 0.27 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 8 | 0.27 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 10 | 0.27 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 10 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 10 | 0.27 |
| (1,1215) | 1:110:A:GLY:HA3 | 1:111:A:TYR:H | 9 | 0.27 |
| (1,1197) | 1:100:A:ILE:HG21 | 1:105:A:ALA:H | 20 | 0.27 |
| (1,1197) | 1:100:A:ILE:HG22 | 1:105:A:ALA:H | 20 | 0.27 |
| (1,1197) | 1:100:A:ILE:HG23 | 1:105:A:ALA:H | 20 | 0.27 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 14 | 0.27 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 12 | 0.27 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 14 | 0.27 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 14 | 0.27 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 14 | 0.27 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 17 | 0.27 |
| (1,1093) | 1:87:A:VAL:HG11 | 1:90:A:MET:H | 14 | 0.27 |
| (1,1093) | 1:87:A:VAL:HG12 | 1:90:A:MET:H | 14 | 0.27 |
| (1,1093) | 1:87:A:VAL:HG13 | 1:90:A:MET:H | 14 | 0.27 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 6 | 0.27 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 6 | 0.27 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 6 | 0.27 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 11 | 0.27 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 11 | 0.27 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 11 | 0.27 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 4 | 0.27 |
| (1,983) | 1:73:A:THR:H | 1:78:A:GLU:HB2 | 1 | 0.27 |
| (1,812) | 1:43:A:GLY:H | 1:44:A:LYS:HB2 | 1 | 0.27 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 14 | 0.27 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 14 | 0.27 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 14 | 0.27 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 1 | 0.27 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 9 | 0.27 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 9 | 0.27 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 9 | 0.27 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 5 | 0.27 |
| (1,775) | 1:34:A:GLY:H | 1:94:A:GLU:HB3 | 4 | 0.27 |
| (1,749) | 1:27:A:GLU:H | 1:27:A:GLU:HG3 | 15 | 0.27 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 19 | 0.27 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 19 | 0.27 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 19 | 0.27 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG21 | 11 | 0.27 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG22 | 11 | 0.27 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG23 | 11 | 0.27 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 20 | 0.27 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG21 | 9 | 0.27 |
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG22 | 9 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,621) | 1:50:A:TYR:HB3 | 1:125:A:VAL:HG23 | 9 | 0.27 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 9 | 0.27 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 13 | 0.27 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB1 | 11 | 0.27 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB2 | 11 | 0.27 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB3 | 11 | 0.27 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 16 | 0.27 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 14 | 0.27 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 16 | 0.27 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 19 | 0.27 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 4 | 0.27 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 4 | 0.27 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 4 | 0.27 |
| (1,425) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 18 | 0.27 |
| (1,421) | 1:91:A:THR:HA | 1:127:A:LEU:HG | 1 | 0.27 |
| (1,391) | 1:46:A:VAL:HG21 | 1:87:A:VAL:HB | 6 | 0.27 |
| (1,391) | 1:46:A:VAL:HG22 | 1:87:A:VAL:HB | 6 | 0.27 |
| (1,391) | 1:46:A:VAL:HG23 | 1:87:A:VAL:HB | 6 | 0.27 |
| (1,378) | 1:81:A:LYS:HA | 1:84:A:ASP:HB3 | 8 | 0.27 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD11 | 18 | 0.27 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD12 | 18 | 0.27 |
| (1,338) | 1:81:A:LYS:HB3 | 1:104:A:LEU:HD13 | 18 | 0.27 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD21 | 20 | 0.27 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD22 | 20 | 0.27 |
| (1,335) | 1:81:A:LYS:HA | 1:104:A:LEU:HD23 | 20 | 0.27 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 1 | 0.27 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 1 | 0.27 |
| (1,309) | 1:80:A:ILE:HA | 1:81:A:LYS:HB2 | 2 | 0.27 |
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 14 | 0.27 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 14 | 0.27 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 14 | 0.27 |
| (1,278) | 1:74:A:LEU:HD11 | 1:87:A:VAL:HB | 17 | 0.27 |
| (1,278) | 1:74:A:LEU:HD12 | 1:87:A:VAL:HB | 17 | 0.27 |
| (1,278) | 1:74:A:LEU:HD13 | 1:87:A:VAL:HB | 17 | 0.27 |
| (1,216) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 17 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,216) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 19 | 0.27 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 16 | 0.27 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 3 | 0.27 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 17 | 0.27 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 1 | 0.27 |
| (1,93) | 1:41:A:GLN:HG3 | 1:44:A:LYS:HG2 | 12 | 0.27 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 7 | 0.27 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG21 | 3 | 0.27 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG22 | 3 | 0.27 |
| (1,79) | 1:40:A:PRO:HD2 | 1:91:A:THR:HG23 | 3 | 0.27 |
| (1,69) | 1:38:A:THR:HG21 | 1:130:A:VAL:HB | 5 | 0.27 |
| (1,69) | 1:38:A:THR:HG22 | 1:130:A:VAL:HB | 5 | 0.27 |
| (1,69) | 1:38:A:THR:HG23 | 1:130:A:VAL:HB | 5 | 0.27 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG21 | 18 | 0.27 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG22 | 18 | 0.27 |
| (1,63) | 1:38:A:THR:HB | 1:91:A:THR:HG23 | 18 | 0.27 |
| (1,48) | 1:34:A:GLY:HA2 | 1:94:A:GLU:HB3 | 6 | 0.27 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 14 | 0.26 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 14 | 0.26 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 14 | 0.26 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 14 | 0.26 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 14 | 0.26 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 14 | 0.26 |
| (1,1631) | 1:109:A:ARG:HB2 | 1:110:A:GLY:H | 17 | 0.26 |
| (1,1631) | 1:109:A:ARG:HB3 | 1:110:A:GLY:H | 17 | 0.26 |
| (1,1624) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 14 | 0.26 |
| (1,1624) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 14 | 0.26 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD11 | 4 | 0.26 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD12 | 4 | 0.26 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD13 | 4 | 0.26 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD11 | 4 | 0.26 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD12 | 4 | 0.26 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD13 | 4 | 0.26 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 17 | 0.26 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 17 | 0.26 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 17 | 0.26 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 17 | 0.26 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 17 | 0.26 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 17 | 0.26 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 2 | 0.26 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 2 | 0.26 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 2 | 0.26 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 2 | 0.26 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 2 | 0.26 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 12 | 0.26 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 12 | 0.26 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 12 | 0.26 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 12 | 0.26 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 12 | 0.26 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 12 | 0.26 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 6 | 0.26 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 6 | 0.26 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 6 | 0.26 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 6 | 0.26 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 6 | 0.26 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 6 | 0.26 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 6 | 0.26 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 6 | 0.26 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 18 | 0.26 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 18 | 0.26 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 10 | 0.26 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 10 | 0.26 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 17 | 0.26 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 10 | 0.26 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 10 | 0.26 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 10 | 0.26 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 14 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 1 | 0.26 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 1 | 0.26 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 1 | 0.26 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 7 | 0.26 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 6 | 0.26 |
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 6 | 0.26 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 6 | 0.26 |
| (1,1197) | 1:100:A:ILE:HG21 | 1:105:A:ALA:H | 6 | 0.26 |
| (1,1197) | 1:100:A:ILE:HG22 | 1:105:A:ALA:H | 6 | 0.26 |
| (1,1197) | 1:100:A:ILE:HG23 | 1:105:A:ALA:H | 6 | 0.26 |
| (1,1174) | 1:102:A:TYR:H | 1:120:A:THR:HB | 2 | 0.26 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 15 | 0.26 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 15 | 0.26 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 15 | 0.26 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 5 | 0.26 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 5 | 0.26 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 5 | 0.26 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 17 | 0.26 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 18 | 0.26 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 9 | 0.26 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 10 | 0.26 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 14 | 0.26 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 14 | 0.26 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 14 | 0.26 |
| (1,972) | 1:70:A:PHE:HD2 | 1:71:A:GLN:H | 15 | 0.26 |
| (1,960) | 1:50:A:TYR:HE2 | 1:70:A:PHE:H | 7 | 0.26 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 1 | 0.26 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 2 | 0.26 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 9 | 0.26 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 2 | 0.26 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 11 | 0.26 |
| (1,859) | 1:50:A:TYR:HD2 | 1:51:A:ASP:H | 17 | 0.26 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 6 | 0.26 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 16 | 0.26 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 8 | 0.26 |
| (1,779) | 1:36:A:GLY:H | 1:91:A:THR:HG21 | 7 | 0.26 |
| (1,779) | 1:36:A:GLY:H | 1:91:A:THR:HG22 | 7 | 0.26 |
| (1,779) | 1:36:A:GLY:H | 1:91:A:THR:HG23 | 7 | 0.26 |
| (1,704) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HA | 16 | 0.26 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 18 | 0.26 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 18 | 0.26 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 18 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,681) | 1:50:A:TYR:H | 1:50:A:TYR:HD2 | 20 | 0.26 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 7 | 0.26 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 7 | 0.26 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 7 | 0.26 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 5 | 0.26 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 9 | 0.26 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 11 | 0.26 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 12 | 0.26 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 12 | 0.26 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 12 | 0.26 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 10 | 0.26 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 3 | 0.26 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 3 | 0.26 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 3 | 0.26 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 20 | 0.26 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD21 | 5 | 0.26 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD22 | 5 | 0.26 |
| (1,509) | 1:81:A:LYS:HE2 | 1:104:A:LEU:HD23 | 5 | 0.26 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB1 | 11 | 0.26 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB2 | 11 | 0.26 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB3 | 11 | 0.26 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB1 | 13 | 0.26 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB2 | 13 | 0.26 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB3 | 13 | 0.26 |
| (1,464) | 1:27:A:GLU:HB2 | 1:99:A:THR:HB | 1 | 0.26 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 7 | 0.26 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 2 | 0.26 |
| (1,414) | 1:90:A:MET:HE1 | 1:126:A:GLU:HA | 4 | 0.26 |
| (1,414) | 1:90:A:MET:HE2 | 1:126:A:GLU:HA | 4 | 0.26 |
| (1,414) | 1:90:A:MET:HE3 | 1:126:A:GLU:HA | 4 | 0.26 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG21 | 19 | 0.26 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG22 | 19 | 0.26 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG23 | 19 | 0.26 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 6 | 0.26 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 6 | 0.26 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 6 | 0.26 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 6 | 0.26 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD11 | 10 | 0.26 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD12 | 10 | 0.26 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD13 | 10 | 0.26 |
| (1,276) | 1:74:A:LEU:HD11 | 1:88:A:ALA:H | 9 | 0.26 |
| (1,276) | 1:74:A:LEU:HD12 | 1:88:A:ALA:H | 9 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,276) | 1:74:A:LEU:HD13 | 1:88:A:ALA:H | 9 | 0.26 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 10 | 0.26 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 10 | 0.26 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 10 | 0.26 |
| (1,266) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 16 | 0.26 |
| (1,266) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 16 | 0.26 |
| (1,266) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 16 | 0.26 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 20 | 0.26 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 11 | 0.26 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 11 | 0.26 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 11 | 0.26 |
| (1,232) | 1:48:A:VAL:H | 1:69:A:PRO:HB3 | 3 | 0.26 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 4 | 0.26 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 12 | 0.26 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 16 | 0.26 |
| (1,225) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 18 | 0.26 |
| (1,216) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 9 | 0.26 |
| (1,212) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 4 | 0.26 |
| (1,212) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 11 | 0.26 |
| (1,212) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 18 | 0.26 |
| (1,212) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 20 | 0.26 |
| (1,211) | 1:49:A:HIS:HB3 | 1:64:A:ARG:HA | 7 | 0.26 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 7 | 0.26 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 11 | 0.26 |
| (1,196) | 1:59:A:GLN:H | 1:59:A:GLN:HG2 | 17 | 0.26 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 9 | 0.26 |
| (1,165) | 1:53:A:ARG:HG2 | 1:60:A:PHE:H | 11 | 0.26 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 16 | 0.26 |
| (1,147) | 1:50:A:TYR:HA | 1:124:A:GLU:HB3 | 16 | 0.26 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 12 | 0.26 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 12 | 0.26 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 12 | 0.26 |
| (1,106) | 1:45:A:LYS:H | 1:45:A:LYS:HE3 | 2 | 0.26 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 1 | 0.26 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 20 | 0.26 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 9 | 0.26 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 9 | 0.26 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 9 | 0.26 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 3 | 0.26 |
| (1,38) | 1:31:A:LEU:HG | 1:32:A:THR:H | 15 | 0.26 |
| (1,29) | 1:27:A:GLU:H | 1:27:A:GLU:HG2 | 14 | 0.26 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 8 | 0.26 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 19 | 0.26 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD2 | 17 | 0.25 |
| (1,1614) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HD3 | 17 | 0.25 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 17 | 0.25 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 17 | 0.25 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 17 | 0.25 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 17 | 0.25 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 17 | 0.25 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 17 | 0.25 |
| (1,1575) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 15 | 0.25 |
| (1,1575) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 15 | 0.25 |
| (1,1575) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 15 | 0.25 |
| (1,1575) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 15 | 0.25 |
| (1,1575) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 15 | 0.25 |
| (1,1575) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 15 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 3 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 3 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 3 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 3 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 3 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 3 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 15 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 15 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 15 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 15 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 15 | 0.25 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 15 | 0.25 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 18 | 0.25 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 18 | 0.25 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 12 | 0.25 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 12 | 0.25 |
| (1,1441) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 1 | 0.25 |
| (1,1441) | 1:53:A:ARG:HD3 | 1:57:A:GLY:HA2 | 1 | 0.25 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 5 | 0.25 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 5 | 0.25 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 5 | 0.25 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 5 | 0.25 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 5 | 0.25 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 5 | 0.25 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 13 | 0.25 |
| (1,1430) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB3 | 13 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 7 | 0.25 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 7 | 0.25 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 10 | 0.25 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 10 | 0.25 |
| (1,1405) | 1:44:A:LYS:HE2 | 1:45:A:LYS:H | 7 | 0.25 |
| (1,1405) | 1:44:A:LYS:HE3 | 1:45:A:LYS:H | 7 | 0.25 |
| (1,1399) | 1:44:A:LYS:HB2 | 1:44:A:LYS:HE2 | 1 | 0.25 |
| (1,1399) | 1:44:A:LYS:HB2 | 1:44:A:LYS:HE3 | 1 | 0.25 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 1 | 0.25 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 1 | 0.25 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 20 | 0.25 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 20 | 0.25 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 3 | 0.25 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 3 | 0.25 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 3 | 0.25 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 19 | 0.25 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 19 | 0.25 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 19 | 0.25 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 11 | 0.25 |
| (1,1213) | 1:109:A:ARG:HB3 | 1:110:A:GLY:H | 17 | 0.25 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 8 | 0.25 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 10 | 0.25 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 1 | 0.25 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 2 | 0.25 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 1 | 0.25 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 1 | 0.25 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 1 | 0.25 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 13 | 0.25 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 7 | 0.25 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 7 | 0.25 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 7 | 0.25 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 20 | 0.25 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 20 | 0.25 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 20 | 0.25 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 19 | 0.25 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 12 | 0.25 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 8 | 0.25 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 8 | 0.25 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 8 | 0.25 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 2 | 0.25 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 2 | 0.25 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 2 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 20 | 0.25 |
| (1,952) | 1:67:A:GLY:H | 1:68:A:LYS:HB2 | 2 | 0.25 |
| (1,951) | 1:67:A:GLY:H | 1:68:A:LYS:HB3 | 9 | 0.25 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 20 | 0.25 |
| (1,912) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 6 | 0.25 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 5 | 0.25 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 8 | 0.25 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 18 | 0.25 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 4 | 0.25 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 4 | 0.25 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 4 | 0.25 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 4 | 0.25 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 16 | 0.25 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 16 | 0.25 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 16 | 0.25 |
| (1,696) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HB3 | 20 | 0.25 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 14 | 0.25 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 13 | 0.25 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 11 | 0.25 |
| (1,643) | 1:49:A:HIS:HD1 | 1:128:A:LEU:HG | 1 | 0.25 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 6 | 0.25 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 1 | 0.25 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 1 | 0.25 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 1 | 0.25 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 10 | 0.25 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 10 | 0.25 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 10 | 0.25 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 12 | 0.25 |
| (1,502) | 1:82:A:GLY:H | 1:104:A:LEU:HG | 7 | 0.25 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 18 | 0.25 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 18 | 0.25 |
| (1,482) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HB2 | 4 | 0.25 |
| (1,482) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HB2 | 4 | 0.25 |
| (1,482) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HB2 | 4 | 0.25 |
| (1,425) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 4 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 7 | 0.25 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 7 | 0.25 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 7 | 0.25 |
| (1,378) | 1:81:A:LYS:HA | 1:84:A:ASP:HB3 | 19 | 0.25 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 5 | 0.25 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 5 | 0.25 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 5 | 0.25 |
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 10 | 0.25 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 10 | 0.25 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 10 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB1 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB2 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB3 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB1 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB2 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB3 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB1 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB2 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB3 | 2 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB1 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB2 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB3 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB1 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB2 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB3 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB1 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB2 | 12 | 0.25 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB3 | 12 | 0.25 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 3 | 0.25 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 9 | 0.25 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 16 | 0.25 |
| (1,212) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 8 | 0.25 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 6 | 0.25 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 4 | 0.25 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 8 | 0.25 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 10 | 0.25 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 10 | 0.25 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 10 | 0.25 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 5 | 0.24 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 5 | 0.24 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 5 | 0.24 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 5 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 5 | 0.24 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 5 | 0.24 |
| (1,1598) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB2 | 19 | 0.24 |
| (1,1598) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB2 | 19 | 0.24 |
| (1,1598) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB2 | 19 | 0.24 |
| (1,1598) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB2 | 19 | 0.24 |
| (1,1598) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB2 | 19 | 0.24 |
| (1,1598) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB2 | 19 | 0.24 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG11 | 2 | 0.24 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG12 | 2 | 0.24 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG13 | 2 | 0.24 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG21 | 2 | 0.24 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG22 | 2 | 0.24 |
| (1,1566) | 1:92:A:LEU:H | 1:130:A:VAL:HG23 | 2 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 6 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 6 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 6 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 6 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 6 | 0.24 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 6 | 0.24 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 14 | 0.24 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 14 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG21 | 17 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG22 | 17 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG23 | 17 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG21 | 17 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG22 | 17 | 0.24 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG23 | 17 | 0.24 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 8 | 0.24 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 8 | 0.24 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 6 | 0.24 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 6 | 0.24 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 4 | 0.24 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 16 | 0.24 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 15 | 0.24 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 15 | 0.24 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 15 | 0.24 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 16 | 0.24 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 16 | 0.24 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 16 | 0.24 |
| (1,1252) | 1:100:A:ILE:HD11 | 1:123:A:PHE:H | 20 | 0.24 |
| (1,1252) | 1:100:A:ILE:HD12 | 1:123:A:PHE:H | 20 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1252) | 1:100:A:ILE:HD13 | 1:123:A:PHE:H | 20 | 0.24 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 19 | 0.24 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 6 | 0.24 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 12 | 0.24 |
| (1,1059) | 1:84:A:ASP:HB2 | 1:85:A:GLN:H | 14 | 0.24 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 10 | 0.24 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 10 | 0.24 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 10 | 0.24 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 12 | 0.24 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 12 | 0.24 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 12 | 0.24 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 3 | 0.24 |
| (1,1036) | 1:79:A:VAL:HB | 1:83:A:TRP:H | 3 | 0.24 |
| (1,1025) | 1:82:A:GLY:H | 1:104:A:LEU:HA | 19 | 0.24 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 6 | 0.24 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 13 | 0.24 |
| (1,858) | 1:50:A:TYR:HD1 | 1:51:A:ASP:H | 3 | 0.24 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 20 | 0.24 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 7 | 0.24 |
| (1,775) | 1:34:A:GLY:H | 1:94:A:GLU:HB3 | 12 | 0.24 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 12 | 0.24 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 12 | 0.24 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 12 | 0.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG21 | 19 | 0.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG22 | 19 | 0.24 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG23 | 19 | 0.24 |
| (1,708) | 1:11:A:THR:HA | 1:12:A:LEU:H | 6 | 0.24 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 20 | 0.24 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 7 | 0.24 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 7 | 0.24 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 7 | 0.24 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 12 | 0.24 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 12 | 0.24 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 12 | 0.24 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 4 | 0.24 |
| (1,623) | 1:95:A:LYS:HB2 | 1:126:A:GLU:HA | 16 | 0.24 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 19 | 0.24 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 19 | 0.24 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 19 | 0.24 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 15 | 0.24 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 16 | 0.24 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 19 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 20 | 0.24 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 17 | 0.24 |
| (1,566) | 1:111:A:TYR:HB2 | 1:115:A:ILE:HB | 12 | 0.24 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB1 | 9 | 0.24 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB2 | 9 | 0.24 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB3 | 9 | 0.24 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB1 | 13 | 0.24 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB2 | 13 | 0.24 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB3 | 13 | 0.24 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 5 | 0.24 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 5 | 0.24 |
| (1,482) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HB2 | 8 | 0.24 |
| (1,482) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HB2 | 8 | 0.24 |
| (1,482) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HB2 | 8 | 0.24 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 8 | 0.24 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 8 | 0.24 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 8 | 0.24 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 8 | 0.24 |
| (1,450) | 1:32:A:THR:HB | 1:95:A:LYS:HE3 | 1 | 0.24 |
| (1,444) | 1:31:A:LEU:HG | 1:95:A:LYS:HB3 | 12 | 0.24 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE1 | 11 | 0.24 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE2 | 11 | 0.24 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE3 | 11 | 0.24 |
| (1,391) | 1:46:A:VAL:HG21 | 1:87:A:VAL:HB | 17 | 0.24 |
| (1,391) | 1:46:A:VAL:HG22 | 1:87:A:VAL:HB | 17 | 0.24 |
| (1,391) | 1:46:A:VAL:HG23 | 1:87:A:VAL:HB | 17 | 0.24 |
| (1,371) | 1:81:A:LYS:HD3 | 1:84:A:ASP:HB2 | 8 | 0.24 |
| (1,354) | 1:82:A:GLY:HA2 | 1:104:A:LEU:HB3 | 4 | 0.24 |
| (1,346) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA3 | 9 | 0.24 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD21 | 2 | 0.24 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD22 | 2 | 0.24 |
| (1,340) | 1:81:A:LYS:HG2 | 1:104:A:LEU:HD23 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG21 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG22 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG23 | 2 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG21 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG22 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG23 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG21 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG22 | 2 | 0.24 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG23 | 2 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 18 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 18 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 18 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 20 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 20 | 0.24 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 20 | 0.24 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB1 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB2 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG21 | 1:76:A:ALA:HB3 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB1 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB2 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG22 | 1:76:A:ALA:HB3 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB1 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB2 | 4 | 0.24 |
| (1,284) | 1:73:A:THR:HG23 | 1:76:A:ALA:HB3 | 4 | 0.24 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 20 | 0.24 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 20 | 0.24 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 20 | 0.24 |
| (1,216) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 3 | 0.24 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 19 | 0.24 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 5 | 0.24 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 11 | 0.24 |
| (1,184) | 1:53:A:ARG:HD3 | 1:57:A:GLY:HA2 | 17 | 0.24 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG21 | 10 | 0.24 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG22 | 10 | 0.24 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG23 | 10 | 0.24 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 7 | 0.24 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 7 | 0.24 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 7 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 5 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 5 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 5 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 6 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 6 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 6 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 17 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 17 | 0.24 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 17 | 0.24 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 10 | 0.24 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 10 | 0.24 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 10 | 0.24 |
| (1,82) | 1:42:A:ALA:HA | 1:74:A:LEU:HB2 | 12 | 0.24 |
| (1,77) | 1:40:A:PRO:HD3 | 1:130:A:VAL:HB | 19 | 0.24 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 7 | 0.24 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 7 | 0.24 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 7 | 0.24 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG21 | 19 | 0.24 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG22 | 19 | 0.24 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG23 | 19 | 0.24 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 5 | 0.24 |
| (1,1619) | 1:103:A:GLN:HG2 | 1:104:A:LEU:H | 3 | 0.23 |
| (1,1619) | 1:103:A:GLN:HG3 | 1:104:A:LEU:H | 3 | 0.23 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 9 | 0.23 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 9 | 0.23 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 9 | 0.23 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 9 | 0.23 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 9 | 0.23 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 9 | 0.23 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 4 | 0.23 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 4 | 0.23 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB2 | 15 | 0.23 |
| (1,1453) | 1:54:A:PHE:HE1 | 1:60:A:PHE:HB3 | 15 | 0.23 |
| (1,1442) | 1:53:A:ARG:HD2 | 1:59:A:GLN:HA | 18 | 0.23 |
| (1,1442) | 1:53:A:ARG:HD3 | 1:59:A:GLN:HA | 18 | 0.23 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD2 | 5 | 0.23 |
| (1,1428) | 1:49:A:HIS:HE1 | 1:69:A:PRO:HD3 | 5 | 0.23 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 1 | 0.23 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 1 | 0.23 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 1 | 0.23 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 1 | 0.23 |
| (1,1380) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 6 | 0.23 |
| (1,1380) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 6 | 0.23 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 15 | 0.23 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 2 | 0.23 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 1 | 0.23 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 20 | 0.23 |
| (1,1215) | 1:110:A:GLY:HA3 | 1:111:A:TYR:H | 16 | 0.23 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 6 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 11 | 0.23 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 9 | 0.23 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 11 | 0.23 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 9 | 0.23 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 16 | 0.23 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 1 | 0.23 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 6 | 0.23 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 7 | 0.23 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 15 | 0.23 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 6 | 0.23 |
| (1,929) | 1:63:A:SER:H | 1:64:A:ARG:HG3 | 19 | 0.23 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 20 | 0.23 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 4 | 0.23 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 9 | 0.23 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 2 | 0.23 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 2 | 0.23 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 2 | 0.23 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 12 | 0.23 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 12 | 0.23 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 12 | 0.23 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 11 | 0.23 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 12 | 0.23 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG21 | 2 | 0.23 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG22 | 2 | 0.23 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG23 | 2 | 0.23 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 11 | 0.23 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 11 | 0.23 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 11 | 0.23 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 1 | 0.23 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 20 | 0.23 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 20 | 0.23 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 20 | 0.23 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 16 | 0.23 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 16 | 0.23 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 16 | 0.23 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB1 | 15 | 0.23 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB2 | 15 | 0.23 |
| (1,580) | 1:115:A:ILE:HD11 | 1:119:A:ALA:HB3 | 15 | 0.23 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB1 | 15 | 0.23 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB2 | 15 | 0.23 |
| (1,580) | 1:115:A:ILE:HD12 | 1:119:A:ALA:HB3 | 15 | 0.23 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB1 | 15 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB2 | 15 | 0.23 |
| (1,580) | 1:115:A:ILE:HD13 | 1:119:A:ALA:HB3 | 15 | 0.23 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 11 | 0.23 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 11 | 0.23 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 11 | 0.23 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 2 | 0.23 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 2 | 0.23 |
| (1,516) | 1:81:A:LYS:H | 1:105:A:ALA:HA | 20 | 0.23 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD11 | 17 | 0.23 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD12 | 17 | 0.23 |
| (1,504) | 1:82:A:GLY:H | 1:104:A:LEU:HD13 | 17 | 0.23 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB1 | 9 | 0.23 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB2 | 9 | 0.23 |
| (1,491) | 1:102:A:TYR:HB3 | 1:105:A:ALA:HB3 | 9 | 0.23 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 15 | 0.23 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 15 | 0.23 |
| (1,482) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HB2 | 10 | 0.23 |
| (1,482) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HB2 | 10 | 0.23 |
| (1,482) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HB2 | 10 | 0.23 |
| (1,462) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 18 | 0.23 |
| (1,462) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 18 | 0.23 |
| (1,462) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 18 | 0.23 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 7 | 0.23 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 7 | 0.23 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 7 | 0.23 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 18 | 0.23 |
| (1,444) | 1:31:A:LEU:HG | 1:95:A:LYS:HB3 | 19 | 0.23 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 19 | 0.23 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 19 | 0.23 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 19 | 0.23 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 19 | 0.23 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 19 | 0.23 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 19 | 0.23 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 11 | 0.23 |
| (1,357) | 1:80:A:ILE:HG13 | 1:83:A:TRP:HB2 | 9 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 5 | 0.23 |
| (1,310) | 1:80:A:ILE:HA | 1:81:A:LYS:HG2 | 7 | 0.23 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD11 | 4 | 0.23 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD12 | 4 | 0.23 |
| (1,305) | 1:79:A:VAL:HB | 1:80:A:ILE:HD13 | 4 | 0.23 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 20 | 0.23 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 10 | 0.23 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 14 | 0.23 |
| (1,227) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 19 | 0.23 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 13 | 0.23 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 19 | 0.23 |
| (1,152) | 1:51:A:ASP:HB2 | 1:124:A:GLU:H | 16 | 0.23 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 8 | 0.23 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 8 | 0.23 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 8 | 0.23 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 13 | 0.23 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 13 | 0.23 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 13 | 0.23 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 10 | 0.23 |
| (1,29) | 1:27:A:GLU:H | 1:27:A:GLU:HG2 | 6 | 0.23 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 11 | 0.23 |
| (1,1624) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG2 | 11 | 0.22 |
| (1,1624) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 11 | 0.22 |
| (1,1619) | 1:103:A:GLN:HG2 | 1:104:A:LEU:H | 15 | 0.22 |
| (1,1619) | 1:103:A:GLN:HG3 | 1:104:A:LEU:H | 15 | 0.22 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG2 | 6 | 0.22 |
| (1,1612) | 1:102:A:TYR:HB2 | 1:108:A:GLU:HG3 | 6 | 0.22 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG11 | 20 | 0.22 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG12 | 20 | 0.22 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG13 | 20 | 0.22 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG21 | 20 | 0.22 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG22 | 20 | 0.22 |
| (1,1608) | 1:99:A:THR:HB | 1:122:A:VAL:HG23 | 20 | 0.22 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 7 | 0.22 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 7 | 0.22 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 7 | 0.22 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 7 | 0.22 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 7 | 0.22 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 7 | 0.22 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 4 | 0.22 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 4 | 0.22 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 4 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 4 | 0.22 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 4 | 0.22 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 4 | 0.22 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 16 | 0.22 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 16 | 0.22 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 1 | 0.22 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 1 | 0.22 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 2 | 0.22 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 2 | 0.22 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 12 | 0.22 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 12 | 0.22 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 19 | 0.22 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 19 | 0.22 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 8 | 0.22 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 8 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD2 | 1:97:A:LEU:HD11 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD2 | 1:97:A:LEU:HD12 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD2 | 1:97:A:LEU:HD13 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD2 | 1:97:A:LEU:HD21 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD2 | 1:97:A:LEU:HD22 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD2 | 1:97:A:LEU:HD23 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD3 | 1:97:A:LEU:HD11 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD3 | 1:97:A:LEU:HD12 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD3 | 1:97:A:LEU:HD13 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD3 | 1:97:A:LEU:HD21 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD3 | 1:97:A:LEU:HD22 | 17 | 0.22 |
| (1,1443) | 1:53:A:ARG:HD3 | 1:97:A:LEU:HD23 | 17 | 0.22 |
| (1,1380) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 13 | 0.22 |
| (1,1380) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 13 | 0.22 |
| (1,1307) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE21 | 6 | 0.22 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 20 | 0.22 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 20 | 0.22 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 20 | 0.22 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 3 | 0.22 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 12 | 0.22 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 15 | 0.22 |
| (1,1197) | 1:100:A:ILE:HG21 | 1:105:A:ALA:H | 10 | 0.22 |
| (1,1197) | 1:100:A:ILE:HG22 | 1:105:A:ALA:H | 10 | 0.22 |
| (1,1197) | 1:100:A:ILE:HG23 | 1:105:A:ALA:H | 10 | 0.22 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 10 | 0.22 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 3 | 0.22 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 14 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 18 | 0.22 |
| (1,1120) | 1:34:A:GLY:HA2 | 1:94:A:GLU:H | 11 | 0.22 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 16 | 0.22 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 16 | 0.22 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 16 | 0.22 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 20 | 0.22 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 7 | 0.22 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 7 | 0.22 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 7 | 0.22 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 20 | 0.22 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 20 | 0.22 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 20 | 0.22 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 14 | 0.22 |
| (1,1047) | 1:84:A:ASP:H | 1:84:A:ASP:HB2 | 14 | 0.22 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 17 | 0.22 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 17 | 0.22 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 17 | 0.22 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 1 | 0.22 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 1 | 0.22 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 1 | 0.22 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 7 | 0.22 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 7 | 0.22 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 7 | 0.22 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 2 | 0.22 |
| (1,977) | 1:47:A:THR:HG21 | 1:71:A:GLN:H | 1 | 0.22 |
| (1,977) | 1:47:A:THR:HG22 | 1:71:A:GLN:H | 1 | 0.22 |
| (1,977) | 1:47:A:THR:HG23 | 1:71:A:GLN:H | 1 | 0.22 |
| (1,903) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB2 | 4 | 0.22 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG11 | 11 | 0.22 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG12 | 11 | 0.22 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG13 | 11 | 0.22 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 7 | 0.22 |
| (1,858) | 1:50:A:TYR:HD1 | 1:51:A:ASP:H | 20 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 1 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 1 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 1 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 4 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 4 | 0.22 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 4 | 0.22 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 13 | 0.22 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 13 | 0.22 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,705) | 1:49:A:HIS:HE1 | 1:64:A:ARG:HA | 5 | 0.22 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD11 | 7 | 0.22 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD12 | 7 | 0.22 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD13 | 7 | 0.22 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 5 | 0.22 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 12 | 0.22 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 14 | 0.22 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 10 | 0.22 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 13 | 0.22 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 12 | 0.22 |
| (1,541) | 1:108:A:GLU:HA | 1:118:A:LYS:HA | 20 | 0.22 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 5 | 0.22 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 10 | 0.22 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD11 | 5 | 0.22 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD12 | 5 | 0.22 |
| (1,511) | 1:81:A:LYS:HD2 | 1:104:A:LEU:HD13 | 5 | 0.22 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 18 | 0.22 |
| (1,481) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HA | 6 | 0.22 |
| (1,481) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HA | 6 | 0.22 |
| (1,481) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HA | 6 | 0.22 |
| (1,470) | 1:100:A:ILE:HB | 1:121:A:LEU:HB2 | 3 | 0.22 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 8 | 0.22 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 8 | 0.22 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 8 | 0.22 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 15 | 0.22 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 15 | 0.22 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 15 | 0.22 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 12 | 0.22 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 12 | 0.22 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 12 | 0.22 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 14 | 0.22 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 14 | 0.22 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 14 | 0.22 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG21 | 16 | 0.22 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG22 | 16 | 0.22 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG23 | 16 | 0.22 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 20 | 0.22 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 20 | 0.22 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 20 | 0.22 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 18 | 0.22 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 8 | 0.22 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 8 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 8 | 0.22 |
| (1,343) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 2 | 0.22 |
| (1,309) | 1:80:A:ILE:HA | 1:81:A:LYS:HB2 | 6 | 0.22 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 17 | 0.22 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 17 | 0.22 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 17 | 0.22 |
| (1,292) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HG2 | 16 | 0.22 |
| (1,292) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HG2 | 16 | 0.22 |
| (1,292) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HG2 | 16 | 0.22 |
| (1,276) | 1:74:A:LEU:HD11 | 1:88:A:ALA:H | 11 | 0.22 |
| (1,276) | 1:74:A:LEU:HD12 | 1:88:A:ALA:H | 11 | 0.22 |
| (1,276) | 1:74:A:LEU:HD13 | 1:88:A:ALA:H | 11 | 0.22 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 17 | 0.22 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 7 | 0.22 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 6 | 0.22 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG21 | 7 | 0.22 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG22 | 7 | 0.22 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG23 | 7 | 0.22 |
| (1,157) | 1:52:A:GLY:HA2 | 1:124:A:GLU:H | 10 | 0.22 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 6 | 0.22 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 7 | 0.22 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 10 | 0.22 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 6 | 0.22 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 18 | 0.22 |
| (1,94) | 1:41:A:GLN:HG2 | 1:44:A:LYS:HG3 | 12 | 0.22 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 5 | 0.22 |
| (1,3) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 11 | 0.22 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 1 | 0.21 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 1 | 0.21 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 1 | 0.21 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 1 | 0.21 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 1 | 0.21 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 1 | 0.21 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 15 | 0.21 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 15 | 0.21 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 15 | 0.21 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 15 | 0.21 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 15 | 0.21 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 15 | 0.21 |
| (1,1404) | 1:44:A:LYS:HD2 | 1:45:A:LYS:H | 18 | 0.21 |
| (1,1404) | 1:44:A:LYS:HD3 | 1:45:A:LYS:H | 18 | 0.21 |
| (1,1399) | 1:44:A:LYS:HB2 | 1:44:A:LYS:HE2 | 2 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1399) | 1:44:A:LYS:HB2 | 1:44:A:LYS:HE3 | 2 | 0.21 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE2 | 18 | 0.21 |
| (1,1396) | 1:41:A:GLN:HE21 | 1:44:A:LYS:HE3 | 18 | 0.21 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE2 | 18 | 0.21 |
| (1,1396) | 1:41:A:GLN:HE22 | 1:44:A:LYS:HE3 | 18 | 0.21 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE2 | 7 | 0.21 |
| (1,1391) | 1:41:A:GLN:HB2 | 1:44:A:LYS:HE3 | 7 | 0.21 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE2 | 7 | 0.21 |
| (1,1391) | 1:41:A:GLN:HB3 | 1:44:A:LYS:HE3 | 7 | 0.21 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 19 | 0.21 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 19 | 0.21 |
| (1,1332) | 1:24:A:ALA:HA | 1:103:A:GLN:HG2 | 8 | 0.21 |
| (1,1332) | 1:24:A:ALA:HA | 1:103:A:GLN:HG3 | 8 | 0.21 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 16 | 0.21 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 16 | 0.21 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 16 | 0.21 |
| (1,1308) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 14 | 0.21 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 16 | 0.21 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 1 | 0.21 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 17 | 0.21 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 13 | 0.21 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 16 | 0.21 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 10 | 0.21 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 1 | 0.21 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 1 | 0.21 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 1 | 0.21 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 13 | 0.21 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 13 | 0.21 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 13 | 0.21 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 8 | 0.21 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 5 | 0.21 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 5 | 0.21 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 5 | 0.21 |
| (1,1029) | 1:82:A:GLY:H | 1:104:A:LEU:HB3 | 4 | 0.21 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 19 | 0.21 |
| (1,1009) | 1:76:A:ALA:H | 1:78:A:GLU:H | 16 | 0.21 |
| (1,1005) | 1:77:A:GLY:H | 1:78:A:GLU:H | 15 | 0.21 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 12 | 0.21 |
| (1,906) | 1:58:A:LYS:HG2 | 1:59:A:GLN:H | 17 | 0.21 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 14 | 0.21 |
| (1,858) | 1:50:A:TYR:HD1 | 1:51:A:ASP:H | 9 | 0.21 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 12 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 12 | 0.21 |
| (1,819) | 1:44:A:LYS:H | 1:44:A:LYS:HG2 | 3 | 0.21 |
| (1,802) | 1:41:A:GLN:H | 1:74:A:LEU:HB3 | 9 | 0.21 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 18 | 0.21 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 18 | 0.21 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 18 | 0.21 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 20 | 0.21 |
| (1,775) | 1:34:A:GLY:H | 1:94:A:GLU:HB3 | 18 | 0.21 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 17 | 0.21 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 17 | 0.21 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 17 | 0.21 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG21 | 17 | 0.21 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG22 | 17 | 0.21 |
| (1,729) | 1:35:A:ASP:H | 1:91:A:THR:HG23 | 17 | 0.21 |
| (1,709) | 1:11:A:THR:HG21 | 1:12:A:LEU:H | 11 | 0.21 |
| (1,709) | 1:11:A:THR:HG22 | 1:12:A:LEU:H | 11 | 0.21 |
| (1,709) | 1:11:A:THR:HG23 | 1:12:A:LEU:H | 11 | 0.21 |
| (1,694) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HD1 | 5 | 0.21 |
| (1,694) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HD1 | 5 | 0.21 |
| (1,694) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HD1 | 5 | 0.21 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 15 | 0.21 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 15 | 0.21 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 15 | 0.21 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG21 | 9 | 0.21 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG22 | 9 | 0.21 |
| (1,667) | 1:106:A:TYR:HE1 | 1:115:A:ILE:HG23 | 9 | 0.21 |
| (1,631) | 1:92:A:LEU:H | 1:127:A:LEU:HG | 14 | 0.21 |
| (1,619) | 1:98:A:PHE:HD1 | 1:125:A:VAL:HG21 | 6 | 0.21 |
| (1,619) | 1:98:A:PHE:HD1 | 1:125:A:VAL:HG22 | 6 | 0.21 |
| (1,619) | 1:98:A:PHE:HD1 | 1:125:A:VAL:HG23 | 6 | 0.21 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 10 | 0.21 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 18 | 0.21 |
| (1,530) | 1:106:A:TYR:HB3 | 1:111:A:TYR:HD2 | 13 | 0.21 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD11 | 15 | 0.21 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD12 | 15 | 0.21 |
| (1,474) | 1:98:A:PHE:HD2 | 1:100:A:ILE:HD13 | 15 | 0.21 |
| (1,449) | 1:32:A:THR:HB | 1:95:A:LYS:HE2 | 1 | 0.21 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE1 | 2 | 0.21 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE2 | 2 | 0.21 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE3 | 2 | 0.21 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 3 | 0.21 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 3 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 3 | 0.21 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 14 | 0.21 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 14 | 0.21 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 14 | 0.21 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG21 | 17 | 0.21 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG22 | 17 | 0.21 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG23 | 17 | 0.21 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 13 | 0.21 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 17 | 0.21 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 17 | 0.21 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 17 | 0.21 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 12 | 0.21 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 12 | 0.21 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 12 | 0.21 |
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 2 | 0.21 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 2 | 0.21 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 2 | 0.21 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 8 | 0.21 |
| (1,166) | 1:53:A:ARG:HG3 | 1:60:A:PHE:H | 18 | 0.21 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 13 | 0.21 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 19 | 0.21 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 5 | 0.21 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 5 | 0.21 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 5 | 0.21 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 10 | 0.21 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 10 | 0.21 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 10 | 0.21 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 3 | 0.21 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 3 | 0.21 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 3 | 0.21 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 19 | 0.21 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB1 | 11 | 0.21 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB2 | 11 | 0.21 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB3 | 11 | 0.21 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 2 | 0.21 |
| (1,1605) | 1:98:A:PHE:HB2 | 1:100:A:ILE:H | 19 | 0.2 |
| (1,1605) | 1:98:A:PHE:HB3 | 1:100:A:ILE:H | 19 | 0.2 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 18 | 0.2 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 18 | 0.2 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 18 | 0.2 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 18 | 0.2 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 18 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 18 | 0.2 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 9 | 0.2 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 9 | 0.2 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 9 | 0.2 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 9 | 0.2 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 9 | 0.2 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 9 | 0.2 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 9 | 0.2 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 9 | 0.2 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 9 | 0.2 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 9 | 0.2 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 9 | 0.2 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 9 | 0.2 |
| (1,1575) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 16 | 0.2 |
| (1,1575) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 16 | 0.2 |
| (1,1575) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 16 | 0.2 |
| (1,1575) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 16 | 0.2 |
| (1,1575) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 16 | 0.2 |
| (1,1575) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 16 | 0.2 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 14 | 0.2 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 14 | 0.2 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 4 | 0.2 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 4 | 0.2 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 8 | 0.2 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 8 | 0.2 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 11 | 0.2 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 11 | 0.2 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 20 | 0.2 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 20 | 0.2 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 4 | 0.2 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 4 | 0.2 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 4 | 0.2 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 4 | 0.2 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 4 | 0.2 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 4 | 0.2 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 19 | 0.2 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 19 | 0.2 |
| (1,1425) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB2 | 1 | 0.2 |
| (1,1425) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB3 | 1 | 0.2 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 15 | 0.2 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 15 | 0.2 |
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG2 | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1386) | 1:41:A:GLN:H | 1:44:A:LYS:HG3 | 20 | 0.2 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 2 | 0.2 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB3 | 2 | 0.2 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG11 | 7 | 0.2 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG12 | 7 | 0.2 |
| (1,1381) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG13 | 7 | 0.2 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG11 | 7 | 0.2 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG12 | 7 | 0.2 |
| (1,1381) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG13 | 7 | 0.2 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG11 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG12 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG13 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG21 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG22 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG21 | 1:130:A:VAL:HG23 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG11 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG12 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG13 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG21 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG22 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG22 | 1:130:A:VAL:HG23 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG11 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG12 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG13 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG21 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG22 | 4 | 0.2 |
| (1,1377) | 1:38:A:THR:HG23 | 1:130:A:VAL:HG23 | 4 | 0.2 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 14 | 0.2 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 14 | 0.2 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 15 | 0.2 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 15 | 0.2 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 1 | 0.2 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 14 | 0.2 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 14 | 0.2 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 14 | 0.2 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 7 | 0.2 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 7 | 0.2 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 7 | 0.2 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 6 | 0.2 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 8 | 0.2 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 4 | 0.2 |
| (1,1179) | 1:102:A:TYR:HE1 | 1:103:A:GLN:H | 18 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 4 | 0.2 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 4 | 0.2 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 4 | 0.2 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD11 | 8 | 0.2 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD12 | 8 | 0.2 |
| (1,1157) | 1:98:A:PHE:H | 1:100:A:ILE:HD13 | 8 | 0.2 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 6 | 0.2 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 6 | 0.2 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 6 | 0.2 |
| (1,1111) | 1:38:A:THR:HG21 | 1:92:A:LEU:H | 9 | 0.2 |
| (1,1111) | 1:38:A:THR:HG22 | 1:92:A:LEU:H | 9 | 0.2 |
| (1,1111) | 1:38:A:THR:HG23 | 1:92:A:LEU:H | 9 | 0.2 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 9 | 0.2 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 2 | 0.2 |
| (1,1069) | 1:86:A:GLY:H | 1:98:A:PHE:HD2 | 19 | 0.2 |
| (1,1065) | 1:79:A:VAL:HG21 | 1:85:A:GLN:H | 16 | 0.2 |
| (1,1065) | 1:79:A:VAL:HG22 | 1:85:A:GLN:H | 16 | 0.2 |
| (1,1065) | 1:79:A:VAL:HG23 | 1:85:A:GLN:H | 16 | 0.2 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 8 | 0.2 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 8 | 0.2 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 8 | 0.2 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG11 | 19 | 0.2 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG12 | 19 | 0.2 |
| (1,986) | 1:73:A:THR:H | 1:79:A:VAL:HG13 | 19 | 0.2 |
| (1,935) | 1:64:A:ARG:H | 1:64:A:ARG:HD2 | 10 | 0.2 |
| (1,896) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB2 | 1 | 0.2 |
| (1,866) | 1:51:A:ASP:H | 1:124:A:GLU:HB3 | 18 | 0.2 |
| (1,862) | 1:50:A:TYR:HB3 | 1:51:A:ASP:H | 17 | 0.2 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 2 | 0.2 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 10 | 0.2 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 14 | 0.2 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 5 | 0.2 |
| (1,799) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 6 | 0.2 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 19 | 0.2 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 19 | 0.2 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 19 | 0.2 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 19 | 0.2 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 19 | 0.2 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 19 | 0.2 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 17 | 0.2 |
| (1,747) | 1:27:A:GLU:H | 1:98:A:PHE:HA | 7 | 0.2 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG21 | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG22 | 20 | 0.2 |
| (1,728) | 1:35:A:ASP:H | 1:38:A:THR:HG23 | 20 | 0.2 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 14 | 0.2 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 14 | 0.2 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 14 | 0.2 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 2 | 0.2 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 2 | 0.2 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 2 | 0.2 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG11 | 8 | 0.2 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG12 | 8 | 0.2 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG13 | 8 | 0.2 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 15 | 0.2 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 15 | 0.2 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 15 | 0.2 |
| (1,624) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB3 | 1 | 0.2 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 8 | 0.2 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 8 | 0.2 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 8 | 0.2 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 4 | 0.2 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 17 | 0.2 |
| (1,557) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HB | 20 | 0.2 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 15 | 0.2 |
| (1,537) | 1:108:A:GLU:HB2 | 1:118:A:LYS:HG2 | 9 | 0.2 |
| (1,528) | 1:80:A:ILE:HG21 | 1:106:A:TYR:HA | 1 | 0.2 |
| (1,528) | 1:80:A:ILE:HG22 | 1:106:A:TYR:HA | 1 | 0.2 |
| (1,528) | 1:80:A:ILE:HG23 | 1:106:A:TYR:HA | 1 | 0.2 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 17 | 0.2 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 17 | 0.2 |
| (1,507) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 17 | 0.2 |
| (1,443) | 1:32:A:THR:HG21 | 1:95:A:LYS:HB3 | 8 | 0.2 |
| (1,443) | 1:32:A:THR:HG22 | 1:95:A:LYS:HB3 | 8 | 0.2 |
| (1,443) | 1:32:A:THR:HG23 | 1:95:A:LYS:HB3 | 8 | 0.2 |
| (1,425) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 15 | 0.2 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB1 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB2 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE1 | 1:96:A:ALA:HB3 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB1 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB2 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE2 | 1:96:A:ALA:HB3 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB1 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB2 | 4 | 0.2 |
| (1,418) | 1:90:A:MET:HE3 | 1:96:A:ALA:HB3 | 4 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,388) | 1:86:A:GLY:HA2 | 1:98:A:PHE:HD2 | 1 | 0.2 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 8 | 0.2 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 8 | 0.2 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 8 | 0.2 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 5 | 0.2 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 11 | 0.2 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 11 | 0.2 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 11 | 0.2 |
| (1,266) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 7 | 0.2 |
| (1,266) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 7 | 0.2 |
| (1,266) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 7 | 0.2 |
| (1,229) | 1:69:A:PRO:HA | 1:128:A:LEU:HG | 15 | 0.2 |
| (1,197) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 10 | 0.2 |
| (1,193) | 1:53:A:ARG:HB3 | 1:59:A:GLN:HA | 9 | 0.2 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 18 | 0.2 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 9 | 0.2 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 8 | 0.2 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 8 | 0.2 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 8 | 0.2 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 14 | 0.2 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 14 | 0.2 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 14 | 0.2 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 17 | 0.2 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 17 | 0.2 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 17 | 0.2 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 14 | 0.2 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 14 | 0.2 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 14 | 0.2 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 4 | 0.2 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 4 | 0.2 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 4 | 0.2 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 7 | 0.2 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 8 | 0.2 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 8 | 0.2 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 8 | 0.2 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 17 | 0.2 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 17 | 0.2 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 17 | 0.2 |
| (1,81) | 1:42:A:ALA:HA | 1:74:A:LEU:H | 3 | 0.2 |
| (1,28) | 1:27:A:GLU:HG2 | 1:99:A:THR:HB | 8 | 0.2 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 20 | 0.2 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 20 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1629) | 1:109:A:ARG:HA | 1:117:A:PRO:HB2 | 17 | 0.19 |
| (1,1629) | 1:109:A:ARG:HA | 1:117:A:PRO:HB3 | 17 | 0.19 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB2 | 2 | 0.19 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB3 | 2 | 0.19 |
| (1,1601) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HG3 | 3 | 0.19 |
| (1,1601) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HG3 | 3 | 0.19 |
| (1,1601) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HG3 | 3 | 0.19 |
| (1,1601) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HG3 | 3 | 0.19 |
| (1,1601) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HG3 | 3 | 0.19 |
| (1,1601) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HG3 | 3 | 0.19 |
| (1,1575) | 1:92:A:LEU:HD11 | 1:130:A:VAL:H | 1 | 0.19 |
| (1,1575) | 1:92:A:LEU:HD12 | 1:130:A:VAL:H | 1 | 0.19 |
| (1,1575) | 1:92:A:LEU:HD13 | 1:130:A:VAL:H | 1 | 0.19 |
| (1,1575) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 1 | 0.19 |
| (1,1575) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 1 | 0.19 |
| (1,1575) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 1 | 0.19 |
| (1,1543) | 1:85:A:GLN:HB2 | 1:98:A:PHE:HD2 | 13 | 0.19 |
| (1,1543) | 1:85:A:GLN:HB3 | 1:98:A:PHE:HD2 | 13 | 0.19 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 7 | 0.19 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 7 | 0.19 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 8 | 0.19 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 8 | 0.19 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD11 | 9 | 0.19 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD12 | 9 | 0.19 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD13 | 9 | 0.19 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD21 | 9 | 0.19 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD22 | 9 | 0.19 |
| (1,1434) | 1:53:A:ARG:HB2 | 1:97:A:LEU:HD23 | 9 | 0.19 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 19 | 0.19 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 19 | 0.19 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 5 | 0.19 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB3 | 5 | 0.19 |
| (1,1380) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 12 | 0.19 |
| (1,1380) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 12 | 0.19 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 5 | 0.19 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 5 | 0.19 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 1 | 0.19 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 1 | 0.19 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 18 | 0.19 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 18 | 0.19 |
| (1,1311) | 1:81:A:LYS:HE3 | 1:85:A:GLN:HE22 | 11 | 0.19 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 11 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 7 | 0.19 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 7 | 0.19 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 7 | 0.19 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 2 | 0.19 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 16 | 0.19 |
| (1,1235) | 1:55:A:PRO:HG3 | 1:120:A:THR:H | 17 | 0.19 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 16 | 0.19 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 16 | 0.19 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 16 | 0.19 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 19 | 0.19 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 19 | 0.19 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 19 | 0.19 |
| (1,1162) | 1:27:A:GLU:HB2 | 1:99:A:THR:H | 1 | 0.19 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 7 | 0.19 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 7 | 0.19 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 7 | 0.19 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 5 | 0.19 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 5 | 0.19 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 5 | 0.19 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 4 | 0.19 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 4 | 0.19 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 4 | 0.19 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 15 | 0.19 |
| (1,1037) | 1:80:A:ILE:HG12 | 1:83:A:TRP:H | 9 | 0.19 |
| (1,1023) | 1:81:A:LYS:H | 1:81:A:LYS:HG3 | 8 | 0.19 |
| (1,1015) | 1:77:A:GLY:H | 1:79:A:VAL:H | 16 | 0.19 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 17 | 0.19 |
| (1,983) | 1:73:A:THR:H | 1:78:A:GLU:HB2 | 13 | 0.19 |
| (1,977) | 1:47:A:THR:HG21 | 1:71:A:GLN:H | 16 | 0.19 |
| (1,977) | 1:47:A:THR:HG22 | 1:71:A:GLN:H | 16 | 0.19 |
| (1,977) | 1:47:A:THR:HG23 | 1:71:A:GLN:H | 16 | 0.19 |
| (1,968) | 1:47:A:THR:HG21 | 1:70:A:PHE:H | 1 | 0.19 |
| (1,968) | 1:47:A:THR:HG22 | 1:70:A:PHE:H | 1 | 0.19 |
| (1,968) | 1:47:A:THR:HG23 | 1:70:A:PHE:H | 1 | 0.19 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 8 | 0.19 |
| (1,862) | 1:50:A:TYR:HB3 | 1:51:A:ASP:H | 20 | 0.19 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 15 | 0.19 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 2 | 0.19 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 6 | 0.19 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 9 | 0.19 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 12 | 0.19 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 16 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 13 | 0.19 |
| (1,745) | 1:27:A:GLU:H | 1:99:A:THR:H | 6 | 0.19 |
| (1,740) | 1:24:A:ALA:HB1 | 1:25:A:GLN:H | 2 | 0.19 |
| (1,740) | 1:24:A:ALA:HB2 | 1:25:A:GLN:H | 2 | 0.19 |
| (1,740) | 1:24:A:ALA:HB3 | 1:25:A:GLN:H | 2 | 0.19 |
| (1,676) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HG | 16 | 0.19 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 1 | 0.19 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 1 | 0.19 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 1 | 0.19 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG11 | 3 | 0.19 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG12 | 3 | 0.19 |
| (1,659) | 1:50:A:TYR:HD1 | 1:79:A:VAL:HG13 | 3 | 0.19 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB1 | 10 | 0.19 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB2 | 10 | 0.19 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB3 | 10 | 0.19 |
| (1,564) | 1:114:A:VAL:HB | 1:115:A:ILE:H | 14 | 0.19 |
| (1,547) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 11 | 0.19 |
| (1,541) | 1:108:A:GLU:HA | 1:118:A:LYS:HA | 17 | 0.19 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 4 | 0.19 |
| (1,468) | 1:27:A:GLU:H | 1:99:A:THR:HG21 | 6 | 0.19 |
| (1,468) | 1:27:A:GLU:H | 1:99:A:THR:HG22 | 6 | 0.19 |
| (1,468) | 1:27:A:GLU:H | 1:99:A:THR:HG23 | 6 | 0.19 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 1 | 0.19 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 1 | 0.19 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 1 | 0.19 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 5 | 0.19 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 18 | 0.19 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 18 | 0.19 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 18 | 0.19 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE1 | 11 | 0.19 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE2 | 11 | 0.19 |
| (1,416) | 1:87:A:VAL:HA | 1:90:A:MET:HE3 | 11 | 0.19 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 18 | 0.19 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 18 | 0.19 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 18 | 0.19 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 20 | 0.19 |
| (1,355) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA2 | 3 | 0.19 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 5 | 0.19 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 12 | 0.19 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 12 | 0.19 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 12 | 0.19 |
| (1,220) | 1:66:A:ARG:HA | 1:66:A:ARG:HD2 | 20 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 20 | 0.19 |
| (1,183) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 4 | 0.19 |
| (1,172) | 1:53:A:ARG:HD3 | 1:59:A:GLN:H | 8 | 0.19 |
| (1,163) | 1:53:A:ARG:HG3 | 1:59:A:GLN:H | 19 | 0.19 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 1 | 0.19 |
| (1,154) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 19 | 0.19 |
| (1,147) | 1:50:A:TYR:HA | 1:124:A:GLU:HB3 | 12 | 0.19 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 1 | 0.19 |
| (1,123) | 1:46:A:VAL:HG11 | 1:130:A:VAL:HB | 5 | 0.19 |
| (1,123) | 1:46:A:VAL:HG12 | 1:130:A:VAL:HB | 5 | 0.19 |
| (1,123) | 1:46:A:VAL:HG13 | 1:130:A:VAL:HB | 5 | 0.19 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG21 | 19 | 0.19 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG22 | 19 | 0.19 |
| (1,74) | 1:40:A:PRO:HB2 | 1:46:A:VAL:HG23 | 19 | 0.19 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 19 | 0.19 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 19 | 0.19 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 19 | 0.19 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 2 | 0.19 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 2 | 0.19 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 2 | 0.19 |
| (1,29) | 1:27:A:GLU:H | 1:27:A:GLU:HG2 | 16 | 0.19 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB1 | 9 | 0.19 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB2 | 9 | 0.19 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB3 | 9 | 0.19 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 18 | 0.19 |
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 15 | 0.18 |
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 15 | 0.18 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 15 | 0.18 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 15 | 0.18 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 15 | 0.18 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 15 | 0.18 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG2 | 17 | 0.18 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG3 | 17 | 0.18 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG2 | 19 | 0.18 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG3 | 19 | 0.18 |
| (1,1595) | 1:97:A:LEU:HD11 | 1:123:A:PHE:HA | 14 | 0.18 |
| (1,1595) | 1:97:A:LEU:HD12 | 1:123:A:PHE:HA | 14 | 0.18 |
| (1,1595) | 1:97:A:LEU:HD13 | 1:123:A:PHE:HA | 14 | 0.18 |
| (1,1595) | 1:97:A:LEU:HD21 | 1:123:A:PHE:HA | 14 | 0.18 |
| (1,1595) | 1:97:A:LEU:HD22 | 1:123:A:PHE:HA | 14 | 0.18 |
| (1,1595) | 1:97:A:LEU:HD23 | 1:123:A:PHE:HA | 14 | 0.18 |
| (1,1550) | 1:86:A:GLY:HA2 | 1:98:A:PHE:HD2 | 17 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1550) | 1:86:A:GLY:HA3 | 1:98:A:PHE:HD2 | 17 | 0.18 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 11 | 0.18 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 11 | 0.18 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 17 | 0.18 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 17 | 0.18 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 17 | 0.18 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 17 | 0.18 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 17 | 0.18 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 17 | 0.18 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 8 | 0.18 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 8 | 0.18 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 12 | 0.18 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 12 | 0.18 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 18 | 0.18 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 18 | 0.18 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 18 | 0.18 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 18 | 0.18 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 14 | 0.18 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 14 | 0.18 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 17 | 0.18 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 17 | 0.18 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 4 | 0.18 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 4 | 0.18 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG21 | 10 | 0.18 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG22 | 10 | 0.18 |
| (1,1461) | 1:55:A:PRO:HD2 | 1:120:A:THR:HG23 | 10 | 0.18 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG21 | 10 | 0.18 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG22 | 10 | 0.18 |
| (1,1461) | 1:55:A:PRO:HD3 | 1:120:A:THR:HG23 | 10 | 0.18 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 18 | 0.18 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 18 | 0.18 |
| (1,1355) | 1:30:A:VAL:HG11 | 1:33:A:PRO:HB3 | 19 | 0.18 |
| (1,1355) | 1:30:A:VAL:HG12 | 1:33:A:PRO:HB3 | 19 | 0.18 |
| (1,1355) | 1:30:A:VAL:HG13 | 1:33:A:PRO:HB3 | 19 | 0.18 |
| (1,1355) | 1:30:A:VAL:HG21 | 1:33:A:PRO:HB3 | 19 | 0.18 |
| (1,1355) | 1:30:A:VAL:HG22 | 1:33:A:PRO:HB3 | 19 | 0.18 |
| (1,1355) | 1:30:A:VAL:HG23 | 1:33:A:PRO:HB3 | 19 | 0.18 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD2 | 12 | 0.18 |
| (1,1326) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HD3 | 12 | 0.18 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD2 | 12 | 0.18 |
| (1,1326) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HD3 | 12 | 0.18 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 8 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 8 | 0.18 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 8 | 0.18 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 4 | 0.18 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 4 | 0.18 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 4 | 0.18 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 5 | 0.18 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 14 | 0.18 |
| (1,1204) | 1:100:A:ILE:HG21 | 1:106:A:TYR:H | 4 | 0.18 |
| (1,1204) | 1:100:A:ILE:HG22 | 1:106:A:TYR:H | 4 | 0.18 |
| (1,1204) | 1:100:A:ILE:HG23 | 1:106:A:TYR:H | 4 | 0.18 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 10 | 0.18 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 2 | 0.18 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 9 | 0.18 |
| (1,1120) | 1:34:A:GLY:HA2 | 1:94:A:GLU:H | 7 | 0.18 |
| (1,1093) | 1:87:A:VAL:HG11 | 1:90:A:MET:H | 20 | 0.18 |
| (1,1093) | 1:87:A:VAL:HG12 | 1:90:A:MET:H | 20 | 0.18 |
| (1,1093) | 1:87:A:VAL:HG13 | 1:90:A:MET:H | 20 | 0.18 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 6 | 0.18 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 6 | 0.18 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 6 | 0.18 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 8 | 0.18 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 8 | 0.18 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 8 | 0.18 |
| (1,1029) | 1:82:A:GLY:H | 1:104:A:LEU:HB3 | 13 | 0.18 |
| (1,1025) | 1:82:A:GLY:H | 1:104:A:LEU:HA | 13 | 0.18 |
| (1,950) | 1:64:A:ARG:HA | 1:67:A:GLY:H | 7 | 0.18 |
| (1,911) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 8 | 0.18 |
| (1,895) | 1:58:A:LYS:H | 1:59:A:GLN:H | 3 | 0.18 |
| (1,887) | 1:53:A:ARG:HB3 | 1:54:A:PHE:H | 4 | 0.18 |
| (1,887) | 1:53:A:ARG:HB3 | 1:54:A:PHE:H | 10 | 0.18 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 18 | 0.18 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 14 | 0.18 |
| (1,812) | 1:43:A:GLY:H | 1:44:A:LYS:HB2 | 4 | 0.18 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 1 | 0.18 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 5 | 0.18 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 11 | 0.18 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 13 | 0.18 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 14 | 0.18 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 15 | 0.18 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 10 | 0.18 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 10 | 0.18 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 8 | 0.18 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 8 | 0.18 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 8 | 0.18 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 3 | 0.18 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 3 | 0.18 |
| (1,709) | 1:11:A:THR:HG21 | 1:12:A:LEU:H | 19 | 0.18 |
| (1,709) | 1:11:A:THR:HG22 | 1:12:A:LEU:H | 19 | 0.18 |
| (1,709) | 1:11:A:THR:HG23 | 1:12:A:LEU:H | 19 | 0.18 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 10 | 0.18 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 10 | 0.18 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 10 | 0.18 |
| (1,679) | 1:50:A:TYR:HB2 | 1:50:A:TYR:HD2 | 17 | 0.18 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG11 | 13 | 0.18 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG12 | 13 | 0.18 |
| (1,660) | 1:72:A:PHE:HB2 | 1:79:A:VAL:HG13 | 13 | 0.18 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG11 | 5 | 0.18 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG12 | 5 | 0.18 |
| (1,654) | 1:47:A:THR:H | 1:130:A:VAL:HG13 | 5 | 0.18 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB1 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB2 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB3 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB1 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB2 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB3 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB1 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB2 | 7 | 0.18 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB3 | 7 | 0.18 |
| (1,632) | 1:93:A:GLY:H | 1:127:A:LEU:HG | 7 | 0.18 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 3 | 0.18 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG11 | 6 | 0.18 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG12 | 6 | 0.18 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG13 | 6 | 0.18 |
| (1,606) | 1:123:A:PHE:HA | 1:124:A:GLU:HB2 | 9 | 0.18 |
| (1,603) | 1:123:A:PHE:H | 1:124:A:GLU:HA | 14 | 0.18 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 3 | 0.18 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 6 | 0.18 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 19 | 0.18 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 19 | 0.18 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 19 | 0.18 |
| (1,571) | 1:117:A:PRO:HA | 1:118:A:LYS:HG3 | 4 | 0.18 |
| (1,544) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 18 | 0.18 |
| (1,543) | 1:108:A:GLU:HA | 1:118:A:LYS:HG2 | 16 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,539) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HA | 13 | 0.18 |
| (1,498) | 1:103:A:GLN:HA | 1:104:A:LEU:HG | 13 | 0.18 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 12 | 0.18 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 12 | 0.18 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 12 | 0.18 |
| (1,449) | 1:32:A:THR:HB | 1:95:A:LYS:HE2 | 8 | 0.18 |
| (1,444) | 1:31:A:LEU:HG | 1:95:A:LYS:HB3 | 13 | 0.18 |
| (1,430) | 1:92:A:LEU:HD21 | 1:129:A:ALA:HA | 17 | 0.18 |
| (1,430) | 1:92:A:LEU:HD22 | 1:129:A:ALA:HA | 17 | 0.18 |
| (1,430) | 1:92:A:LEU:HD23 | 1:129:A:ALA:HA | 17 | 0.18 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD21 | 3 | 0.18 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD22 | 3 | 0.18 |
| (1,339) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HD23 | 3 | 0.18 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 4 | 0.18 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 10 | 0.18 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 10 | 0.18 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 10 | 0.18 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 19 | 0.18 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 7 | 0.18 |
| (1,183) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 19 | 0.18 |
| (1,160) | 1:53:A:ARG:HB2 | 1:59:A:GLN:HA | 4 | 0.18 |
| (1,146) | 1:49:A:HIS:HD2 | 1:50:A:TYR:HA | 11 | 0.18 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 18 | 0.18 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 18 | 0.18 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 18 | 0.18 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 3 | 0.18 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 19 | 0.18 |
| (1,107) | 1:46:A:VAL:HA | 1:129:A:ALA:HB1 | 3 | 0.18 |
| (1,107) | 1:46:A:VAL:HA | 1:129:A:ALA:HB2 | 3 | 0.18 |
| (1,107) | 1:46:A:VAL:HA | 1:129:A:ALA:HB3 | 3 | 0.18 |
| (1,105) | 1:45:A:LYS:H | 1:45:A:LYS:HE2 | 20 | 0.18 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 4 | 0.18 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 4 | 0.18 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 4 | 0.18 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB1 | 14 | 0.18 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB2 | 14 | 0.18 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB3 | 14 | 0.18 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 17 | 0.18 |
| (1,8) | 1:23:A:SER:HA | 1:24:A:ALA:HB1 | 12 | 0.18 |
| (1,8) | 1:23:A:SER:HA | 1:24:A:ALA:HB2 | 12 | 0.18 |
| (1,8) | 1:23:A:SER:HA | 1:24:A:ALA:HB3 | 12 | 0.18 |
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 20 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 20 | 0.17 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 20 | 0.17 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 20 | 0.17 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 20 | 0.17 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 20 | 0.17 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB2 | 14 | 0.17 |
| (1,1613) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HB3 | 14 | 0.17 |
| (1,1605) | 1:98:A:PHE:HB2 | 1:100:A:ILE:H | 11 | 0.17 |
| (1,1605) | 1:98:A:PHE:HB3 | 1:100:A:ILE:H | 11 | 0.17 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 11 | 0.17 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 11 | 0.17 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 11 | 0.17 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 11 | 0.17 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 11 | 0.17 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 11 | 0.17 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 11 | 0.17 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 11 | 0.17 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 11 | 0.17 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 11 | 0.17 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 11 | 0.17 |
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 11 | 0.17 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 18 | 0.17 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 18 | 0.17 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 18 | 0.17 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 18 | 0.17 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 18 | 0.17 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 18 | 0.17 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG11 | 11 | 0.17 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG12 | 11 | 0.17 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG13 | 11 | 0.17 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG11 | 11 | 0.17 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG12 | 11 | 0.17 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG13 | 11 | 0.17 |
| (1,1511) | 1:70:A:PHE:HB2 | 1:71:A:GLN:H | 17 | 0.17 |
| (1,1511) | 1:70:A:PHE:HB3 | 1:71:A:GLN:H | 17 | 0.17 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 4 | 0.17 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 4 | 0.17 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD2 | 18 | 0.17 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD3 | 18 | 0.17 |
| (1,1475) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 15 | 0.17 |
| (1,1475) | 1:59:A:GLN:HG3 | 1:61:A:ASP:H | 15 | 0.17 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 19 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 19 | 0.17 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 19 | 0.17 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 19 | 0.17 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 19 | 0.17 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 19 | 0.17 |
| (1,1425) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB2 | 18 | 0.17 |
| (1,1425) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB3 | 18 | 0.17 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 7 | 0.17 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB3 | 7 | 0.17 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 2 | 0.17 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 2 | 0.17 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 4 | 0.17 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 10 | 0.17 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 7 | 0.17 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 19 | 0.17 |
| (1,1298) | 1:92:A:LEU:HG | 1:130:A:VAL:H | 10 | 0.17 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 10 | 0.17 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 10 | 0.17 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 10 | 0.17 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 12 | 0.17 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 12 | 0.17 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 12 | 0.17 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 1 | 0.17 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 1 | 0.17 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 1 | 0.17 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 4 | 0.17 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 15 | 0.17 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 18 | 0.17 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 13 | 0.17 |
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 13 | 0.17 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 13 | 0.17 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG21 | 3 | 0.17 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG22 | 3 | 0.17 |
| (1,1220) | 1:111:A:TYR:H | 1:115:A:ILE:HG23 | 3 | 0.17 |
| (1,1204) | 1:100:A:ILE:HG21 | 1:106:A:TYR:H | 13 | 0.17 |
| (1,1204) | 1:100:A:ILE:HG22 | 1:106:A:TYR:H | 13 | 0.17 |
| (1,1204) | 1:100:A:ILE:HG23 | 1:106:A:TYR:H | 13 | 0.17 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 15 | 0.17 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 18 | 0.17 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 5 | 0.17 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 19 | 0.17 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1093) | 1:87:A:VAL:HG11 | 1:90:A:MET:H | 18 | 0.17 |
| (1,1093) | 1:87:A:VAL:HG12 | 1:90:A:MET:H | 18 | 0.17 |
| (1,1093) | 1:87:A:VAL:HG13 | 1:90:A:MET:H | 18 | 0.17 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 19 | 0.17 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 19 | 0.17 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 19 | 0.17 |
| (1,1005) | 1:77:A:GLY:H | 1:78:A:GLU:H | 3 | 0.17 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 14 | 0.17 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 17 | 0.17 |
| (1,977) | 1:47:A:THR:HG21 | 1:71:A:GLN:H | 15 | 0.17 |
| (1,977) | 1:47:A:THR:HG22 | 1:71:A:GLN:H | 15 | 0.17 |
| (1,977) | 1:47:A:THR:HG23 | 1:71:A:GLN:H | 15 | 0.17 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 5 | 0.17 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 10 | 0.17 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 11 | 0.17 |
| (1,902) | 1:59:A:GLN:HE22 | 1:62:A:SER:HB3 | 6 | 0.17 |
| (1,808) | 1:43:A:GLY:H | 1:74:A:LEU:H | 14 | 0.17 |
| (1,808) | 1:43:A:GLY:H | 1:74:A:LEU:H | 15 | 0.17 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 2 | 0.17 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 6 | 0.17 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 6 | 0.17 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 6 | 0.17 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG21 | 3 | 0.17 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG22 | 3 | 0.17 |
| (1,793) | 1:39:A:LYS:H | 1:91:A:THR:HG23 | 3 | 0.17 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 19 | 0.17 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 12 | 0.17 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 19 | 0.17 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG21 | 18 | 0.17 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG22 | 18 | 0.17 |
| (1,730) | 1:35:A:ASP:H | 1:37:A:VAL:HG23 | 18 | 0.17 |
| (1,702) | 1:80:A:ILE:HG21 | 1:83:A:TRP:HE3 | 8 | 0.17 |
| (1,702) | 1:80:A:ILE:HG22 | 1:83:A:TRP:HE3 | 8 | 0.17 |
| (1,702) | 1:80:A:ILE:HG23 | 1:83:A:TRP:HE3 | 8 | 0.17 |
| (1,700) | 1:79:A:VAL:HB | 1:83:A:TRP:HE3 | 20 | 0.17 |
| (1,680) | 1:50:A:TYR:HB3 | 1:50:A:TYR:HD1 | 5 | 0.17 |
| (1,668) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HG21 | 4 | 0.17 |
| (1,668) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HG22 | 4 | 0.17 |
| (1,668) | 1:110:A:GLY:HA3 | 1:115:A:ILE:HG23 | 4 | 0.17 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG11 | 17 | 0.17 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG12 | 17 | 0.17 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG13 | 17 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB1 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB2 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB3 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB1 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB2 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB3 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB1 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB2 | 10 | 0.17 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB3 | 10 | 0.17 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD11 | 18 | 0.17 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD12 | 18 | 0.17 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD13 | 18 | 0.17 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG11 | 1 | 0.17 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG12 | 1 | 0.17 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG13 | 1 | 0.17 |
| (1,608) | 1:97:A:LEU:HG | 1:124:A:GLU:HG3 | 19 | 0.17 |
| (1,603) | 1:123:A:PHE:H | 1:124:A:GLU:HA | 18 | 0.17 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 5 | 0.17 |
| (1,582) | 1:55:A:PRO:HG2 | 1:120:A:THR:HB | 8 | 0.17 |
| (1,519) | 1:80:A:ILE:HB | 1:105:A:ALA:HA | 13 | 0.17 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 7 | 0.17 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 7 | 0.17 |
| (1,506) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 7 | 0.17 |
| (1,498) | 1:103:A:GLN:HA | 1:104:A:LEU:HG | 14 | 0.17 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB1 | 1 | 0.17 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB2 | 1 | 0.17 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB3 | 1 | 0.17 |
| (1,482) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HB2 | 19 | 0.17 |
| (1,482) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HB2 | 19 | 0.17 |
| (1,482) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HB2 | 19 | 0.17 |
| (1,481) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HA | 1 | 0.17 |
| (1,481) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HA | 1 | 0.17 |
| (1,481) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HA | 1 | 0.17 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 17 | 0.17 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 17 | 0.17 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 17 | 0.17 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 19 | 0.17 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 19 | 0.17 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 19 | 0.17 |
| (1,457) | 1:29:A:LYS:H | 1:97:A:LEU:HB2 | 8 | 0.17 |
| (1,457) | 1:29:A:LYS:H | 1:97:A:LEU:HB2 | 10 | 0.17 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB1 | 7 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB2 | 7 | 0.17 |
| (1,455) | 1:30:A:VAL:HB | 1:96:A:ALA:HB3 | 7 | 0.17 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 15 | 0.17 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 15 | 0.17 |
| (1,410) | 1:90:A:MET:HE1 | 1:96:A:ALA:H | 4 | 0.17 |
| (1,410) | 1:90:A:MET:HE2 | 1:96:A:ALA:H | 4 | 0.17 |
| (1,410) | 1:90:A:MET:HE3 | 1:96:A:ALA:H | 4 | 0.17 |
| (1,394) | 1:74:A:LEU:HD11 | 1:88:A:ALA:HA | 14 | 0.17 |
| (1,394) | 1:74:A:LEU:HD12 | 1:88:A:ALA:HA | 14 | 0.17 |
| (1,394) | 1:74:A:LEU:HD13 | 1:88:A:ALA:HA | 14 | 0.17 |
| (1,388) | 1:86:A:GLY:HA2 | 1:98:A:PHE:HD2 | 13 | 0.17 |
| (1,383) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 8 | 0.17 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 6 | 0.17 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 6 | 0.17 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 6 | 0.17 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 14 | 0.17 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 18 | 0.17 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG21 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG22 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD11 | 1:100:A:ILE:HG23 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG21 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG22 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD12 | 1:100:A:ILE:HG23 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG21 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG22 | 13 | 0.17 |
| (1,315) | 1:80:A:ILE:HD13 | 1:100:A:ILE:HG23 | 13 | 0.17 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 6 | 0.17 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 6 | 0.17 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 6 | 0.17 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 14 | 0.17 |
| (1,240) | 1:47:A:THR:HG21 | 1:69:A:PRO:HG3 | 12 | 0.17 |
| (1,240) | 1:47:A:THR:HG22 | 1:69:A:PRO:HG3 | 12 | 0.17 |
| (1,240) | 1:47:A:THR:HG23 | 1:69:A:PRO:HG3 | 12 | 0.17 |
| (1,209) | 1:64:A:ARG:HA | 1:68:A:LYS:H | 9 | 0.17 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 6 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 11 | 0.17 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 11 | 0.17 |
| (1,162) | 1:53:A:ARG:HG2 | 1:59:A:GLN:H | 16 | 0.17 |
| (1,123) | 1:46:A:VAL:HG11 | 1:130:A:VAL:HB | 17 | 0.17 |
| (1,123) | 1:46:A:VAL:HG12 | 1:130:A:VAL:HB | 17 | 0.17 |
| (1,123) | 1:46:A:VAL:HG13 | 1:130:A:VAL:HB | 17 | 0.17 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 16 | 0.17 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 19 | 0.17 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 19 | 0.17 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 19 | 0.17 |
| (1,72) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 10 | 0.17 |
| (1,65) | 1:38:A:THR:HG21 | 1:130:A:VAL:H | 18 | 0.17 |
| (1,65) | 1:38:A:THR:HG22 | 1:130:A:VAL:H | 18 | 0.17 |
| (1,65) | 1:38:A:THR:HG23 | 1:130:A:VAL:H | 18 | 0.17 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 2 | 0.17 |
| (1,29) | 1:27:A:GLU:H | 1:27:A:GLU:HG2 | 17 | 0.17 |
| (1,29) | 1:27:A:GLU:H | 1:27:A:GLU:HG2 | 20 | 0.17 |
| (1,2) | 1:28:A:LYS:HB2 | 1:30:A:VAL:H | 18 | 0.17 |
| (1,1648) | 1:121:A:LEU:HD11 | 1:123:A:PHE:HD1 | 8 | 0.16 |
| (1,1648) | 1:121:A:LEU:HD12 | 1:123:A:PHE:HD1 | 8 | 0.16 |
| (1,1648) | 1:121:A:LEU:HD13 | 1:123:A:PHE:HD1 | 8 | 0.16 |
| (1,1648) | 1:121:A:LEU:HD21 | 1:123:A:PHE:HD1 | 8 | 0.16 |
| (1,1648) | 1:121:A:LEU:HD22 | 1:123:A:PHE:HD1 | 8 | 0.16 |
| (1,1648) | 1:121:A:LEU:HD23 | 1:123:A:PHE:HD1 | 8 | 0.16 |
| (1,1584) | 1:95:A:LYS:HG2 | 1:124:A:GLU:HB3 | 8 | 0.16 |
| (1,1584) | 1:95:A:LYS:HG3 | 1:124:A:GLU:HB3 | 8 | 0.16 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD11 | 3 | 0.16 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD12 | 3 | 0.16 |
| (1,1546) | 1:85:A:GLN:HE21 | 1:104:A:LEU:HD13 | 3 | 0.16 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD11 | 3 | 0.16 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD12 | 3 | 0.16 |
| (1,1546) | 1:85:A:GLN:HE22 | 1:104:A:LEU:HD13 | 3 | 0.16 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 2 | 0.16 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 2 | 0.16 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 2 | 0.16 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 2 | 0.16 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 2 | 0.16 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 2 | 0.16 |
| (1,1511) | 1:70:A:PHE:HB2 | 1:71:A:GLN:H | 4 | 0.16 |
| (1,1511) | 1:70:A:PHE:HB3 | 1:71:A:GLN:H | 4 | 0.16 |
| (1,1505) | 1:66:A:ARG:HG2 | 1:68:A:LYS:H | 1 | 0.16 |
| (1,1505) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1460) | 1:55:A:PRO:HG3 | 1:122:A:VAL:HG11 | 15 | 0.16 |
| (1,1460) | 1:55:A:PRO:HG3 | 1:122:A:VAL:HG12 | 15 | 0.16 |
| (1,1460) | 1:55:A:PRO:HG3 | 1:122:A:VAL:HG13 | 15 | 0.16 |
| (1,1460) | 1:55:A:PRO:HG3 | 1:122:A:VAL:HG21 | 15 | 0.16 |
| (1,1460) | 1:55:A:PRO:HG3 | 1:122:A:VAL:HG22 | 15 | 0.16 |
| (1,1460) | 1:55:A:PRO:HG3 | 1:122:A:VAL:HG23 | 15 | 0.16 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 14 | 0.16 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB3 | 14 | 0.16 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 9 | 0.16 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 17 | 0.16 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 17 | 0.16 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 17 | 0.16 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 5 | 0.16 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 17 | 0.16 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 17 | 0.16 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 17 | 0.16 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 20 | 0.16 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 20 | 0.16 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 20 | 0.16 |
| (1,1218) | 1:111:A:TYR:H | 1:111:A:TYR:HB3 | 13 | 0.16 |
| (1,1214) | 1:111:A:TYR:H | 1:115:A:ILE:H | 12 | 0.16 |
| (1,1197) | 1:100:A:ILE:HG21 | 1:105:A:ALA:H | 19 | 0.16 |
| (1,1197) | 1:100:A:ILE:HG22 | 1:105:A:ALA:H | 19 | 0.16 |
| (1,1197) | 1:100:A:ILE:HG23 | 1:105:A:ALA:H | 19 | 0.16 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB1 | 11 | 0.16 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB2 | 11 | 0.16 |
| (1,1175) | 1:102:A:TYR:H | 1:105:A:ALA:HB3 | 11 | 0.16 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 20 | 0.16 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 1 | 0.16 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 1 | 0.16 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 1 | 0.16 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 16 | 0.16 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 16 | 0.16 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 16 | 0.16 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 11 | 0.16 |
| (1,1041) | 1:80:A:ILE:HG21 | 1:83:A:TRP:H | 14 | 0.16 |
| (1,1041) | 1:80:A:ILE:HG22 | 1:83:A:TRP:H | 14 | 0.16 |
| (1,1041) | 1:80:A:ILE:HG23 | 1:83:A:TRP:H | 14 | 0.16 |
| (1,952) | 1:67:A:GLY:H | 1:68:A:LYS:HB2 | 20 | 0.16 |
| (1,858) | 1:50:A:TYR:HD1 | 1:51:A:ASP:H | 10 | 0.16 |
| (1,836) | 1:47:A:THR:H | 1:128:A:LEU:H | 3 | 0.16 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 17 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 3 | 0.16 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 4 | 0.16 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 7 | 0.16 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 20 | 0.16 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 8 | 0.16 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 8 | 0.16 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 8 | 0.16 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 4 | 0.16 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 4 | 0.16 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 4 | 0.16 |
| (1,775) | 1:34:A:GLY:H | 1:94:A:GLU:HB3 | 15 | 0.16 |
| (1,695) | 1:83:A:TRP:HZ2 | 1:123:A:PHE:HD1 | 1 | 0.16 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 4 | 0.16 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 4 | 0.16 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 4 | 0.16 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 4 | 0.16 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG11 | 9 | 0.16 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG12 | 9 | 0.16 |
| (1,661) | 1:72:A:PHE:HB3 | 1:79:A:VAL:HG13 | 9 | 0.16 |
| (1,653) | 1:38:A:THR:HB | 1:130:A:VAL:HB | 5 | 0.16 |
| (1,630) | 1:127:A:LEU:HG | 1:129:A:ALA:HA | 8 | 0.16 |
| (1,624) | 1:49:A:HIS:HB3 | 1:126:A:GLU:HB3 | 18 | 0.16 |
| (1,603) | 1:123:A:PHE:H | 1:124:A:GLU:HA | 10 | 0.16 |
| (1,601) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB2 | 13 | 0.16 |
| (1,601) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB2 | 13 | 0.16 |
| (1,601) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB2 | 13 | 0.16 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 7 | 0.16 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 9 | 0.16 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 13 | 0.16 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 14 | 0.16 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 15 | 0.16 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB1 | 2 | 0.16 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB2 | 2 | 0.16 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB3 | 2 | 0.16 |
| (1,482) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HB2 | 6 | 0.16 |
| (1,482) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HB2 | 6 | 0.16 |
| (1,482) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HB2 | 6 | 0.16 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 10 | 0.16 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 10 | 0.16 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 10 | 0.16 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 13 | 0.16 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 13 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 13 | 0.16 |
| (1,375) | 1:74:A:LEU:HD11 | 1:84:A:ASP:HB3 | 1 | 0.16 |
| (1,375) | 1:74:A:LEU:HD12 | 1:84:A:ASP:HB3 | 1 | 0.16 |
| (1,375) | 1:74:A:LEU:HD13 | 1:84:A:ASP:HB3 | 1 | 0.16 |
| (1,370) | 1:81:A:LYS:HA | 1:84:A:ASP:HB2 | 14 | 0.16 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 14 | 0.16 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 14 | 0.16 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 14 | 0.16 |
| (1,343) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 18 | 0.16 |
| (1,333) | 1:81:A:LYS:HA | 1:81:A:LYS:HD3 | 19 | 0.16 |
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 17 | 0.16 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 17 | 0.16 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 17 | 0.16 |
| (1,283) | 1:73:A:THR:HG21 | 1:76:A:ALA:HA | 6 | 0.16 |
| (1,283) | 1:73:A:THR:HG22 | 1:76:A:ALA:HA | 6 | 0.16 |
| (1,283) | 1:73:A:THR:HG23 | 1:76:A:ALA:HA | 6 | 0.16 |
| (1,216) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 14 | 0.16 |
| (1,160) | 1:53:A:ARG:HB2 | 1:59:A:GLN:HA | 19 | 0.16 |
| (1,158) | 1:52:A:GLY:HA2 | 1:123:A:PHE:HD1 | 19 | 0.16 |
| (1,156) | 1:51:A:ASP:HA | 1:124:A:GLU:H | 14 | 0.16 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 14 | 0.16 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 14 | 0.16 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 14 | 0.16 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 11 | 0.16 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 11 | 0.16 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 11 | 0.16 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 12 | 0.16 |
| (1,103) | 1:45:A:LYS:HG2 | 1:46:A:VAL:H | 4 | 0.16 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 5 | 0.16 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 5 | 0.16 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 5 | 0.16 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 18 | 0.16 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 18 | 0.16 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 18 | 0.16 |
| (1,42) | 1:33:A:PRO:HA | 1:94:A:GLU:HG2 | 9 | 0.16 |
| (1,1631) | 1:109:A:ARG:HB2 | 1:110:A:GLY:H | 15 | 0.15 |
| (1,1631) | 1:109:A:ARG:HB3 | 1:110:A:GLY:H | 15 | 0.15 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG2 | 15 | 0.15 |
| (1,1627) | 1:109:A:ARG:HA | 1:109:A:ARG:HG3 | 15 | 0.15 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD11 | 17 | 0.15 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD12 | 17 | 0.15 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD13 | 17 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD21 | 17 | 0.15 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD22 | 17 | 0.15 |
| (1,1620) | 1:106:A:TYR:HE2 | 1:121:A:LEU:HD23 | 17 | 0.15 |
| (1,1599) | 1:97:A:LEU:HD11 | 1:124:A:GLU:HB3 | 16 | 0.15 |
| (1,1599) | 1:97:A:LEU:HD12 | 1:124:A:GLU:HB3 | 16 | 0.15 |
| (1,1599) | 1:97:A:LEU:HD13 | 1:124:A:GLU:HB3 | 16 | 0.15 |
| (1,1599) | 1:97:A:LEU:HD21 | 1:124:A:GLU:HB3 | 16 | 0.15 |
| (1,1599) | 1:97:A:LEU:HD22 | 1:124:A:GLU:HB3 | 16 | 0.15 |
| (1,1599) | 1:97:A:LEU:HD23 | 1:124:A:GLU:HB3 | 16 | 0.15 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 2 | 0.15 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 2 | 0.15 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 2 | 0.15 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 2 | 0.15 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 2 | 0.15 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 2 | 0.15 |
| (1,1493) | 1:64:A:ARG:HG2 | 1:65:A:SER:HA | 16 | 0.15 |
| (1,1493) | 1:64:A:ARG:HG3 | 1:65:A:SER:HA | 16 | 0.15 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 17 | 0.15 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 17 | 0.15 |
| (1,1441) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 3 | 0.15 |
| (1,1441) | 1:53:A:ARG:HD3 | 1:57:A:GLY:HA2 | 3 | 0.15 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG2 | 18 | 0.15 |
| (1,1439) | 1:53:A:ARG:HG3 | 1:59:A:GLN:HG3 | 18 | 0.15 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB2 | 12 | 0.15 |
| (1,1336) | 1:25:A:GLN:H | 1:26:A:LEU:HB3 | 12 | 0.15 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG2 | 9 | 0.15 |
| (1,1331) | 1:24:A:ALA:HA | 1:25:A:GLN:HG3 | 9 | 0.15 |
| (1,1308) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 3 | 0.15 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 15 | 0.15 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB1 | 17 | 0.15 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB2 | 17 | 0.15 |
| (1,1304) | 1:71:A:GLN:HE22 | 1:129:A:ALA:HB3 | 17 | 0.15 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 8 | 0.15 |
| (1,1301) | 1:71:A:GLN:HA | 1:71:A:GLN:HE21 | 16 | 0.15 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 14 | 0.15 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 14 | 0.15 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 14 | 0.15 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 6 | 0.15 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 6 | 0.15 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 6 | 0.15 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 19 | 0.15 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 19 | 0.15 |
| (1,1276) | 1:96:A:ALA:H | 1:127:A:LEU:H | 20 | 0.15 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG11 | 6 | 0.15 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG12 | 6 | 0.15 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG13 | 6 | 0.15 |
| (1,1218) | 1:111:A:TYR:H | 1:111:A:TYR:HB3 | 5 | 0.15 |
| (1,1218) | 1:111:A:TYR:H | 1:111:A:TYR:HB3 | 15 | 0.15 |
| (1,1218) | 1:111:A:TYR:H | 1:111:A:TYR:HB3 | 17 | 0.15 |
| (1,1187) | 1:104:A:LEU:H | 1:107:A:GLY:H | 7 | 0.15 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 8 | 0.15 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 6 | 0.15 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 18 | 0.15 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 10 | 0.15 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 2 | 0.15 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 2 | 0.15 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 2 | 0.15 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 17 | 0.15 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 17 | 0.15 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 17 | 0.15 |
| (1,1050) | 1:80:A:ILE:HG12 | 1:84:A:ASP:H | 12 | 0.15 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD11 | 9 | 0.15 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD12 | 9 | 0.15 |
| (1,1038) | 1:83:A:TRP:H | 1:104:A:LEU:HD13 | 9 | 0.15 |
| (1,1037) | 1:80:A:ILE:HG12 | 1:83:A:TRP:H | 6 | 0.15 |
| (1,1017) | 1:76:A:ALA:HB1 | 1:79:A:VAL:H | 16 | 0.15 |
| (1,1017) | 1:76:A:ALA:HB2 | 1:79:A:VAL:H | 16 | 0.15 |
| (1,1017) | 1:76:A:ALA:HB3 | 1:79:A:VAL:H | 16 | 0.15 |
| (1,1006) | 1:77:A:GLY:H | 1:78:A:GLU:HB2 | 19 | 0.15 |
| (1,1005) | 1:77:A:GLY:H | 1:78:A:GLU:H | 18 | 0.15 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB1 | 12 | 0.15 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB2 | 12 | 0.15 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB3 | 12 | 0.15 |
| (1,966) | 1:69:A:PRO:HB3 | 1:70:A:PHE:H | 9 | 0.15 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 4 | 0.15 |
| (1,824) | 1:44:A:LYS:HB3 | 1:45:A:LYS:H | 15 | 0.15 |
| (1,820) | 1:44:A:LYS:H | 1:44:A:LYS:HG3 | 10 | 0.15 |
| (1,812) | 1:43:A:GLY:H | 1:44:A:LYS:HB2 | 3 | 0.15 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 10 | 0.15 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 19 | 0.15 |
| (1,797) | 1:41:A:GLN:H | 1:41:A:GLN:HG2 | 10 | 0.15 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG11 | 10 | 0.15 |
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG12 | 10 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,794) | 1:39:A:LYS:H | 1:130:A:VAL:HG13 | 10 | 0.15 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 14 | 0.15 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 14 | 0.15 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 14 | 0.15 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 16 | 0.15 |
| (1,775) | 1:34:A:GLY:H | 1:94:A:GLU:HB3 | 2 | 0.15 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG21 | 3 | 0.15 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG22 | 3 | 0.15 |
| (1,693) | 1:83:A:TRP:HD1 | 1:100:A:ILE:HG23 | 3 | 0.15 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 18 | 0.15 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 18 | 0.15 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 18 | 0.15 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 8 | 0.15 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 8 | 0.15 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 8 | 0.15 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB1 | 19 | 0.15 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB2 | 19 | 0.15 |
| (1,648) | 1:47:A:THR:H | 1:129:A:ALA:HB3 | 19 | 0.15 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 2 | 0.15 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB1 | 17 | 0.15 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB2 | 17 | 0.15 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB3 | 17 | 0.15 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 11 | 0.15 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 18 | 0.15 |
| (1,555) | 1:106:A:TYR:HB3 | 1:110:A:GLY:HA2 | 19 | 0.15 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 13 | 0.15 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG21 | 16 | 0.15 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG22 | 16 | 0.15 |
| (1,532) | 1:106:A:TYR:HB2 | 1:115:A:ILE:HG23 | 16 | 0.15 |
| (1,481) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HA | 19 | 0.15 |
| (1,481) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HA | 19 | 0.15 |
| (1,481) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HA | 19 | 0.15 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 2 | 0.15 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 2 | 0.15 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 2 | 0.15 |
| (1,457) | 1:29:A:LYS:H | 1:97:A:LEU:HB2 | 13 | 0.15 |
| (1,415) | 1:90:A:MET:HE1 | 1:94:A:GLU:HA | 13 | 0.15 |
| (1,415) | 1:90:A:MET:HE2 | 1:94:A:GLU:HA | 13 | 0.15 |
| (1,415) | 1:90:A:MET:HE3 | 1:94:A:GLU:HA | 13 | 0.15 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 15 | 0.15 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 15 | 0.15 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,395) | 1:40:A:PRO:HG2 | 1:88:A:ALA:HA | 6 | 0.15 |
| (1,376) | 1:81:A:LYS:HG2 | 1:84:A:ASP:HB3 | 6 | 0.15 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 2 | 0.15 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 7 | 0.15 |
| (1,355) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA2 | 6 | 0.15 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG21 | 17 | 0.15 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG22 | 17 | 0.15 |
| (1,353) | 1:82:A:GLY:HA2 | 1:100:A:ILE:HG23 | 17 | 0.15 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG21 | 13 | 0.15 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG22 | 13 | 0.15 |
| (1,349) | 1:82:A:GLY:HA3 | 1:100:A:ILE:HG23 | 13 | 0.15 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD11 | 8 | 0.15 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD12 | 8 | 0.15 |
| (1,334) | 1:81:A:LYS:HA | 1:104:A:LEU:HD13 | 8 | 0.15 |
| (1,328) | 1:80:A:ILE:HG13 | 1:83:A:TRP:H | 11 | 0.15 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 6 | 0.15 |
| (1,242) | 1:68:A:LYS:H | 1:69:A:PRO:HD2 | 7 | 0.15 |
| (1,228) | 1:47:A:THR:HG21 | 1:69:A:PRO:HA | 15 | 0.15 |
| (1,228) | 1:47:A:THR:HG22 | 1:69:A:PRO:HA | 15 | 0.15 |
| (1,228) | 1:47:A:THR:HG23 | 1:69:A:PRO:HA | 15 | 0.15 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 19 | 0.15 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 8 | 0.15 |
| (1,192) | 1:59:A:GLN:HA | 1:61:A:ASP:H | 2 | 0.15 |
| (1,160) | 1:53:A:ARG:HB2 | 1:59:A:GLN:HA | 12 | 0.15 |
| (1,153) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 16 | 0.15 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 4 | 0.15 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 4 | 0.15 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 4 | 0.15 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG11 | 18 | 0.15 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG12 | 18 | 0.15 |
| (1,151) | 1:50:A:TYR:HB2 | 1:125:A:VAL:HG13 | 18 | 0.15 |
| (1,100) | 1:45:A:LYS:HB3 | 1:46:A:VAL:HA | 16 | 0.15 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 9 | 0.15 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD21 | 14 | 0.15 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD22 | 14 | 0.15 |
| (1,85) | 1:42:A:ALA:HA | 1:74:A:LEU:HD23 | 14 | 0.15 |
| (1,1619) | 1:103:A:GLN:HG2 | 1:104:A:LEU:H | 8 | 0.14 |
| (1,1619) | 1:103:A:GLN:HG3 | 1:104:A:LEU:H | 8 | 0.14 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD11 | 13 | 0.14 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD12 | 13 | 0.14 |
| (1,1606) | 1:98:A:PHE:HB2 | 1:100:A:ILE:HD13 | 13 | 0.14 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD11 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD12 | 13 | 0.14 |
| (1,1606) | 1:98:A:PHE:HB3 | 1:100:A:ILE:HD13 | 13 | 0.14 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 19 | 0.14 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 19 | 0.14 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 19 | 0.14 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 19 | 0.14 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 19 | 0.14 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 19 | 0.14 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 6 | 0.14 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 6 | 0.14 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 6 | 0.14 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 6 | 0.14 |
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 6 | 0.14 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 6 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 7 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 7 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 7 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 7 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 7 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 7 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 10 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 10 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 10 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 10 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 10 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 10 | 0.14 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 13 | 0.14 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 13 | 0.14 |
| (1,1501) | 1:66:A:ARG:HA | 1:66:A:ARG:HG2 | 6 | 0.14 |
| (1,1501) | 1:66:A:ARG:HA | 1:66:A:ARG:HG3 | 6 | 0.14 |
| (1,1446) | 1:54:A:PHE:H | 1:58:A:LYS:HB2 | 17 | 0.14 |
| (1,1446) | 1:54:A:PHE:H | 1:58:A:LYS:HB3 | 17 | 0.14 |
| (1,1441) | 1:53:A:ARG:HD2 | 1:57:A:GLY:HA2 | 4 | 0.14 |
| (1,1441) | 1:53:A:ARG:HD3 | 1:57:A:GLY:HA2 | 4 | 0.14 |
| (1,1327) | 1:19:A:PRO:HG2 | 1:56:A:ASP:H | 11 | 0.14 |
| (1,1327) | 1:19:A:PRO:HG3 | 1:56:A:ASP:H | 11 | 0.14 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 6 | 0.14 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 12 | 0.14 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB1 | 19 | 0.14 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB2 | 19 | 0.14 |
| (1,1302) | 1:71:A:GLN:HE21 | 1:129:A:ALA:HB3 | 19 | 0.14 |
| (1,1300) | 1:92:A:LEU:HD21 | 1:130:A:VAL:H | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1300) | 1:92:A:LEU:HD22 | 1:130:A:VAL:H | 9 | 0.14 |
| (1,1300) | 1:92:A:LEU:HD23 | 1:130:A:VAL:H | 9 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 8 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 8 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 8 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 15 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 15 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 15 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 18 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 18 | 0.14 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 18 | 0.14 |
| (1,1281) | 1:95:A:LYS:HB2 | 1:127:A:LEU:H | 2 | 0.14 |
| (1,1276) | 1:96:A:ALA:H | 1:127:A:LEU:H | 17 | 0.14 |
| (1,1201) | 1:106:A:TYR:H | 1:106:A:TYR:HD2 | 12 | 0.14 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 1 | 0.14 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 3 | 0.14 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 20 | 0.14 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 4 | 0.14 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 11 | 0.14 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 19 | 0.14 |
| (1,1121) | 1:34:A:GLY:HA3 | 1:94:A:GLU:H | 2 | 0.14 |
| (1,1120) | 1:34:A:GLY:HA2 | 1:94:A:GLU:H | 16 | 0.14 |
| (1,1118) | 1:34:A:GLY:H | 1:94:A:GLU:H | 18 | 0.14 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 11 | 0.14 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 11 | 0.14 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 11 | 0.14 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 14 | 0.14 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 14 | 0.14 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 14 | 0.14 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 2 | 0.14 |
| (1,1053) | 1:80:A:ILE:HG21 | 1:84:A:ASP:H | 2 | 0.14 |
| (1,1053) | 1:80:A:ILE:HG22 | 1:84:A:ASP:H | 2 | 0.14 |
| (1,1053) | 1:80:A:ILE:HG23 | 1:84:A:ASP:H | 2 | 0.14 |
| (1,1036) | 1:79:A:VAL:HB | 1:83:A:TRP:H | 16 | 0.14 |
| (1,977) | 1:47:A:THR:HG21 | 1:71:A:GLN:H | 6 | 0.14 |
| (1,977) | 1:47:A:THR:HG22 | 1:71:A:GLN:H | 6 | 0.14 |
| (1,977) | 1:47:A:THR:HG23 | 1:71:A:GLN:H | 6 | 0.14 |
| (1,965) | 1:69:A:PRO:HG3 | 1:70:A:PHE:H | 19 | 0.14 |
| (1,887) | 1:53:A:ARG:HB3 | 1:54:A:PHE:H | 15 | 0.14 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 9 | 0.14 |
| (1,786) | 1:38:A:THR:H | 1:91:A:THR:HA | 17 | 0.14 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,690) | 1:83:A:TRP:HD1 | 1:123:A:PHE:HD2 | 8 | 0.14 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 6 | 0.14 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 6 | 0.14 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 6 | 0.14 |
| (1,681) | 1:50:A:TYR:H | 1:50:A:TYR:HD2 | 16 | 0.14 |
| (1,680) | 1:50:A:TYR:HB3 | 1:50:A:TYR:HD1 | 17 | 0.14 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG21 | 16 | 0.14 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG22 | 16 | 0.14 |
| (1,666) | 1:111:A:TYR:HD2 | 1:115:A:ILE:HG23 | 16 | 0.14 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG11 | 2 | 0.14 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG12 | 2 | 0.14 |
| (1,616) | 1:50:A:TYR:HA | 1:125:A:VAL:HG13 | 2 | 0.14 |
| (1,602) | 1:100:A:ILE:HD11 | 1:123:A:PHE:HB3 | 7 | 0.14 |
| (1,602) | 1:100:A:ILE:HD12 | 1:123:A:PHE:HB3 | 7 | 0.14 |
| (1,602) | 1:100:A:ILE:HD13 | 1:123:A:PHE:HB3 | 7 | 0.14 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 8 | 0.14 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 14 | 0.14 |
| (1,563) | 1:114:A:VAL:H | 1:114:A:VAL:HB | 20 | 0.14 |
| (1,554) | 1:106:A:TYR:HB2 | 1:110:A:GLY:HA2 | 17 | 0.14 |
| (1,528) | 1:80:A:ILE:HG21 | 1:106:A:TYR:HA | 11 | 0.14 |
| (1,528) | 1:80:A:ILE:HG22 | 1:106:A:TYR:HA | 11 | 0.14 |
| (1,528) | 1:80:A:ILE:HG23 | 1:106:A:TYR:HA | 11 | 0.14 |
| (1,470) | 1:100:A:ILE:HB | 1:121:A:LEU:HB2 | 18 | 0.14 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 9 | 0.14 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 9 | 0.14 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 9 | 0.14 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 19 | 0.14 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD11 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD12 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG21 | 1:92:A:LEU:HD13 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD11 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD12 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG22 | 1:92:A:LEU:HD13 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD11 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD12 | 4 | 0.14 |
| (1,428) | 1:38:A:THR:HG23 | 1:92:A:LEU:HD13 | 4 | 0.14 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 11 | 0.14 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 11 | 0.14 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 11 | 0.14 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 16 | 0.14 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 16 | 0.14 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 16 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 20 | 0.14 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 20 | 0.14 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 20 | 0.14 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE1 | 2 | 0.14 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE2 | 2 | 0.14 |
| (1,412) | 1:90:A:MET:H | 1:90:A:MET:HE3 | 2 | 0.14 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 18 | 0.14 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 18 | 0.14 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 18 | 0.14 |
| (1,377) | 1:81:A:LYS:HD3 | 1:84:A:ASP:HB3 | 19 | 0.14 |
| (1,364) | 1:80:A:ILE:HD11 | 1:83:A:TRP:HA | 4 | 0.14 |
| (1,364) | 1:80:A:ILE:HD12 | 1:83:A:TRP:HA | 4 | 0.14 |
| (1,364) | 1:80:A:ILE:HD13 | 1:83:A:TRP:HA | 4 | 0.14 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 17 | 0.14 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 17 | 0.14 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 17 | 0.14 |
| (1,303) | 1:50:A:TYR:HE1 | 1:79:A:VAL:HB | 14 | 0.14 |
| (1,265) | 1:42:A:ALA:H | 1:74:A:LEU:HB3 | 8 | 0.14 |
| (1,258) | 1:44:A:LYS:H | 1:73:A:THR:HG21 | 6 | 0.14 |
| (1,258) | 1:44:A:LYS:H | 1:73:A:THR:HG22 | 6 | 0.14 |
| (1,258) | 1:44:A:LYS:H | 1:73:A:THR:HG23 | 6 | 0.14 |
| (1,235) | 1:69:A:PRO:HB2 | 1:128:A:LEU:HG | 5 | 0.14 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 6 | 0.14 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 8 | 0.14 |
| (1,231) | 1:68:A:LYS:H | 1:69:A:PRO:HA | 18 | 0.14 |
| (1,229) | 1:69:A:PRO:HA | 1:128:A:LEU:HG | 16 | 0.14 |
| (1,194) | 1:53:A:ARG:HG2 | 1:59:A:GLN:HA | 15 | 0.14 |
| (1,185) | 1:53:A:ARG:HB3 | 1:57:A:GLY:HA2 | 18 | 0.14 |
| (1,177) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG3 | 17 | 0.14 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG21 | 15 | 0.14 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG22 | 15 | 0.14 |
| (1,174) | 1:55:A:PRO:HB3 | 1:120:A:THR:HG23 | 15 | 0.14 |
| (1,160) | 1:53:A:ARG:HB2 | 1:59:A:GLN:HA | 8 | 0.14 |
| (1,157) | 1:52:A:GLY:HA2 | 1:124:A:GLU:H | 19 | 0.14 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 3 | 0.14 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 3 | 0.14 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 3 | 0.14 |
| (1,121) | 1:46:A:VAL:HG11 | 1:130:A:VAL:H | 2 | 0.14 |
| (1,121) | 1:46:A:VAL:HG12 | 1:130:A:VAL:H | 2 | 0.14 |
| (1,121) | 1:46:A:VAL:HG13 | 1:130:A:VAL:H | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD11 | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD12 | 2 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD13 | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD11 | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD12 | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD13 | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD11 | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD12 | 2 | 0.14 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD13 | 2 | 0.14 |
| (1,114) | 1:46:A:VAL:HG21 | 1:47:A:THR:H | 3 | 0.14 |
| (1,114) | 1:46:A:VAL:HG22 | 1:47:A:THR:H | 3 | 0.14 |
| (1,114) | 1:46:A:VAL:HG23 | 1:47:A:THR:H | 3 | 0.14 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB1 | 18 | 0.14 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB2 | 18 | 0.14 |
| (1,110) | 1:46:A:VAL:HB | 1:129:A:ALA:HB3 | 18 | 0.14 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 14 | 0.14 |
| (1,95) | 1:41:A:GLN:HG3 | 1:44:A:LYS:HG3 | 19 | 0.14 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG21 | 5 | 0.14 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG22 | 5 | 0.14 |
| (1,84) | 1:42:A:ALA:HA | 1:73:A:THR:HG23 | 5 | 0.14 |
| (1,29) | 1:27:A:GLU:H | 1:27:A:GLU:HG2 | 2 | 0.14 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 3 | 0.14 |
| (1,22) | 1:27:A:GLU:HB3 | 1:99:A:THR:HB | 7 | 0.14 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB1 | 16 | 0.14 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB2 | 16 | 0.14 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB3 | 16 | 0.14 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG11 | 20 | 0.13 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG12 | 20 | 0.13 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG13 | 20 | 0.13 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG21 | 20 | 0.13 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG22 | 20 | 0.13 |
| (1,1537) | 1:85:A:GLN:H | 1:87:A:VAL:HG23 | 20 | 0.13 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 9 | 0.13 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 9 | 0.13 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 19 | 0.13 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 19 | 0.13 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD2 | 4 | 0.13 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD3 | 4 | 0.13 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 5 | 0.13 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 5 | 0.13 |
| (1,1474) | 1:59:A:GLN:HG2 | 1:60:A:PHE:H | 1 | 0.13 |
| (1,1474) | 1:59:A:GLN:HG3 | 1:60:A:PHE:H | 1 | 0.13 |
| (1,1440) | 1:53:A:ARG:HD2 | 1:57:A:GLY:H | 20 | 0.13 |
| (1,1440) | 1:53:A:ARG:HD3 | 1:57:A:GLY:H | 20 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD11 | 18 | 0.13 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD12 | 18 | 0.13 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD13 | 18 | 0.13 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD21 | 18 | 0.13 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD22 | 18 | 0.13 |
| (1,1437) | 1:53:A:ARG:HB3 | 1:97:A:LEU:HD23 | 18 | 0.13 |
| (1,1414) | 1:45:A:LYS:HG2 | 1:73:A:THR:HA | 6 | 0.13 |
| (1,1414) | 1:45:A:LYS:HG3 | 1:73:A:THR:HA | 6 | 0.13 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 4 | 0.13 |
| (1,1384) | 1:41:A:GLN:H | 1:41:A:GLN:HB3 | 4 | 0.13 |
| (1,1380) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 9 | 0.13 |
| (1,1380) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 9 | 0.13 |
| (1,1328) | 1:19:A:PRO:HG2 | 1:56:A:ASP:HA | 18 | 0.13 |
| (1,1328) | 1:19:A:PRO:HG3 | 1:56:A:ASP:HA | 18 | 0.13 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 6 | 0.13 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 6 | 0.13 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 6 | 0.13 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 20 | 0.13 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 20 | 0.13 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 20 | 0.13 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 3 | 0.13 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 3 | 0.13 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 3 | 0.13 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 16 | 0.13 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 16 | 0.13 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 16 | 0.13 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 14 | 0.13 |
| (1,1204) | 1:100:A:ILE:HG21 | 1:106:A:TYR:H | 17 | 0.13 |
| (1,1204) | 1:100:A:ILE:HG22 | 1:106:A:TYR:H | 17 | 0.13 |
| (1,1204) | 1:100:A:ILE:HG23 | 1:106:A:TYR:H | 17 | 0.13 |
| (1,1199) | 1:80:A:ILE:HG21 | 1:105:A:ALA:H | 5 | 0.13 |
| (1,1199) | 1:80:A:ILE:HG22 | 1:105:A:ALA:H | 5 | 0.13 |
| (1,1199) | 1:80:A:ILE:HG23 | 1:105:A:ALA:H | 5 | 0.13 |
| (1,1195) | 1:80:A:ILE:HB | 1:105:A:ALA:H | 20 | 0.13 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 9 | 0.13 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 12 | 0.13 |
| (1,1120) | 1:34:A:GLY:HA2 | 1:94:A:GLU:H | 6 | 0.13 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 11 | 0.13 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 11 | 0.13 |
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 11 | 0.13 |
| (1,1116) | 1:92:A:LEU:HD11 | 1:93:A:GLY:H | 19 | 0.13 |
| (1,1116) | 1:92:A:LEU:HD12 | 1:93:A:GLY:H | 19 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1116) | 1:92:A:LEU:HD13 | 1:93:A:GLY:H | 19 | 0.13 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 7 | 0.13 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 7 | 0.13 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 7 | 0.13 |
| (1,1084) | 1:89:A:THR:H | 1:90:A:MET:HG3 | 8 | 0.13 |
| (1,1065) | 1:79:A:VAL:HG21 | 1:85:A:GLN:H | 4 | 0.13 |
| (1,1065) | 1:79:A:VAL:HG22 | 1:85:A:GLN:H | 4 | 0.13 |
| (1,1065) | 1:79:A:VAL:HG23 | 1:85:A:GLN:H | 4 | 0.13 |
| (1,923) | 1:71:A:GLN:HE21 | 1:72:A:PHE:H | 12 | 0.13 |
| (1,910) | 1:55:A:PRO:HA | 1:57:A:GLY:H | 19 | 0.13 |
| (1,909) | 1:56:A:ASP:HA | 1:57:A:GLY:H | 14 | 0.13 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG11 | 6 | 0.13 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG12 | 6 | 0.13 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG13 | 6 | 0.13 |
| (1,862) | 1:50:A:TYR:HB3 | 1:51:A:ASP:H | 10 | 0.13 |
| (1,836) | 1:47:A:THR:H | 1:128:A:LEU:H | 16 | 0.13 |
| (1,813) | 1:43:A:GLY:H | 1:74:A:LEU:HG | 17 | 0.13 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD21 | 15 | 0.13 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD22 | 15 | 0.13 |
| (1,805) | 1:42:A:ALA:H | 1:74:A:LEU:HD23 | 15 | 0.13 |
| (1,802) | 1:41:A:GLN:H | 1:74:A:LEU:HB3 | 7 | 0.13 |
| (1,799) | 1:40:A:PRO:HB2 | 1:41:A:GLN:H | 13 | 0.13 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 9 | 0.13 |
| (1,682) | 1:50:A:TYR:HE2 | 1:70:A:PHE:HB2 | 18 | 0.13 |
| (1,679) | 1:50:A:TYR:HB2 | 1:50:A:TYR:HD2 | 5 | 0.13 |
| (1,670) | 1:115:A:ILE:HG21 | 1:119:A:ALA:HB1 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG21 | 1:119:A:ALA:HB2 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG21 | 1:119:A:ALA:HB3 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG22 | 1:119:A:ALA:HB1 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG22 | 1:119:A:ALA:HB2 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG22 | 1:119:A:ALA:HB3 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG23 | 1:119:A:ALA:HB1 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG23 | 1:119:A:ALA:HB2 | 9 | 0.13 |
| (1,670) | 1:115:A:ILE:HG23 | 1:119:A:ALA:HB3 | 9 | 0.13 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 17 | 0.13 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 17 | 0.13 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 17 | 0.13 |
| (1,629) | 1:92:A:LEU:HA | 1:127:A:LEU:HG | 14 | 0.13 |
| (1,598) | 1:123:A:PHE:HB3 | 1:124:A:GLU:HA | 7 | 0.13 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 10 | 0.13 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB1 | 15 | 0.13 |
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB2 | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,579) | 1:102:A:TYR:HB2 | 1:119:A:ALA:HB3 | 15 | 0.13 |
| (1,548) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HG3 | 19 | 0.13 |
| (1,542) | 1:108:A:GLU:HA | 1:118:A:LYS:HG3 | 12 | 0.13 |
| (1,500) | 1:81:A:LYS:HB2 | 1:104:A:LEU:HA | 6 | 0.13 |
| (1,498) | 1:103:A:GLN:HA | 1:104:A:LEU:HG | 16 | 0.13 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD11 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD12 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HD13 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD11 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD12 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HD13 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD11 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD12 | 2 | 0.13 |
| (1,483) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HD13 | 2 | 0.13 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 18 | 0.13 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 18 | 0.13 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 18 | 0.13 |
| (1,457) | 1:29:A:LYS:H | 1:97:A:LEU:HB2 | 18 | 0.13 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB1 | 16 | 0.13 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB2 | 16 | 0.13 |
| (1,454) | 1:94:A:GLU:HG2 | 1:96:A:ALA:HB3 | 16 | 0.13 |
| (1,411) | 1:90:A:MET:HE1 | 1:127:A:LEU:H | 16 | 0.13 |
| (1,411) | 1:90:A:MET:HE2 | 1:127:A:LEU:H | 16 | 0.13 |
| (1,411) | 1:90:A:MET:HE3 | 1:127:A:LEU:H | 16 | 0.13 |
| (1,378) | 1:81:A:LYS:HA | 1:84:A:ASP:HB3 | 9 | 0.13 |
| (1,369) | 1:83:A:TRP:H | 1:84:A:ASP:HB2 | 12 | 0.13 |
| (1,365) | 1:79:A:VAL:HG21 | 1:83:A:TRP:HA | 15 | 0.13 |
| (1,365) | 1:79:A:VAL:HG22 | 1:83:A:TRP:HA | 15 | 0.13 |
| (1,365) | 1:79:A:VAL:HG23 | 1:83:A:TRP:HA | 15 | 0.13 |
| (1,343) | 1:66:A:ARG:HG3 | 1:68:A:LYS:H | 20 | 0.13 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 5 | 0.13 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 5 | 0.13 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 5 | 0.13 |
| (1,333) | 1:81:A:LYS:HA | 1:81:A:LYS:HD3 | 3 | 0.13 |
| (1,328) | 1:80:A:ILE:HG13 | 1:83:A:TRP:H | 13 | 0.13 |
| (1,326) | 1:80:A:ILE:HG13 | 1:104:A:LEU:HB3 | 1 | 0.13 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG21 | 10 | 0.13 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG22 | 10 | 0.13 |
| (1,320) | 1:80:A:ILE:HG21 | 1:100:A:ILE:HG23 | 10 | 0.13 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG21 | 10 | 0.13 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG22 | 10 | 0.13 |
| (1,320) | 1:80:A:ILE:HG22 | 1:100:A:ILE:HG23 | 10 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG21 | 10 | 0.13 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG22 | 10 | 0.13 |
| (1,320) | 1:80:A:ILE:HG23 | 1:100:A:ILE:HG23 | 10 | 0.13 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD11 | 3 | 0.13 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD12 | 3 | 0.13 |
| (1,299) | 1:79:A:VAL:HA | 1:80:A:ILE:HD13 | 3 | 0.13 |
| (1,280) | 1:74:A:LEU:HG | 1:75:A:GLY:HA3 | 14 | 0.13 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD21 | 3 | 0.13 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD22 | 3 | 0.13 |
| (1,267) | 1:43:A:GLY:H | 1:74:A:LEU:HD23 | 3 | 0.13 |
| (1,229) | 1:69:A:PRO:HA | 1:128:A:LEU:HG | 18 | 0.13 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 17 | 0.13 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 14 | 0.13 |
| (1,179) | 1:54:A:PHE:HB2 | 1:55:A:PRO:HD3 | 15 | 0.13 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 20 | 0.13 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 20 | 0.13 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 20 | 0.13 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 1 | 0.13 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 7 | 0.13 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD11 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD12 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG21 | 1:74:A:LEU:HD13 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD11 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD12 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG22 | 1:74:A:LEU:HD13 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD11 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD12 | 15 | 0.13 |
| (1,119) | 1:46:A:VAL:HG23 | 1:74:A:LEU:HD13 | 15 | 0.13 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 5 | 0.13 |
| (1,93) | 1:41:A:GLN:HG3 | 1:44:A:LYS:HG2 | 13 | 0.13 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 2 | 0.13 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 2 | 0.13 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 2 | 0.13 |
| (1,89) | 1:42:A:ALA:HB1 | 1:74:A:LEU:HA | 3 | 0.13 |
| (1,89) | 1:42:A:ALA:HB2 | 1:74:A:LEU:HA | 3 | 0.13 |
| (1,89) | 1:42:A:ALA:HB3 | 1:74:A:LEU:HA | 3 | 0.13 |
| (1,72) | 1:40:A:PRO:HB3 | 1:41:A:GLN:H | 13 | 0.13 |
| (1,70) | 1:38:A:THR:HG21 | 1:92:A:LEU:HG | 14 | 0.13 |
| (1,70) | 1:38:A:THR:HG22 | 1:92:A:LEU:HG | 14 | 0.13 |
| (1,70) | 1:38:A:THR:HG23 | 1:92:A:LEU:HG | 14 | 0.13 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 4 | 0.13 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 2 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 2 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 2 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 2 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 2 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 2 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 6 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 6 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 6 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 6 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 6 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 6 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 12 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 12 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 12 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 12 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 12 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 12 | 0.12 |
| (1,1622) | 1:108:A:GLU:HA | 1:118:A:LYS:HB2 | 13 | 0.12 |
| (1,1622) | 1:108:A:GLU:HA | 1:118:A:LYS:HB3 | 13 | 0.12 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 7 | 0.12 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 7 | 0.12 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG11 | 16 | 0.12 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG12 | 16 | 0.12 |
| (1,1525) | 1:78:A:GLU:HG2 | 1:79:A:VAL:HG13 | 16 | 0.12 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG11 | 16 | 0.12 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG12 | 16 | 0.12 |
| (1,1525) | 1:78:A:GLU:HG3 | 1:79:A:VAL:HG13 | 16 | 0.12 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 8 | 0.12 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 8 | 0.12 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 8 | 0.12 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 8 | 0.12 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 8 | 0.12 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 8 | 0.12 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 9 | 0.12 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 9 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG11 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG12 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG13 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG21 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG22 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB2 | 1:114:A:VAL:HG23 | 20 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG11 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG12 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG13 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG21 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG22 | 20 | 0.12 |
| (1,1478) | 1:60:A:PHE:HB3 | 1:114:A:VAL:HG23 | 20 | 0.12 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA2 | 4 | 0.12 |
| (1,1427) | 1:49:A:HIS:HE1 | 1:67:A:GLY:HA3 | 4 | 0.12 |
| (1,1284) | 1:127:A:LEU:H | 1:127:A:LEU:HG | 1 | 0.12 |
| (1,1284) | 1:127:A:LEU:H | 1:127:A:LEU:HG | 4 | 0.12 |
| (1,1276) | 1:96:A:ALA:H | 1:127:A:LEU:H | 12 | 0.12 |
| (1,1250) | 1:123:A:PHE:H | 1:123:A:PHE:HB3 | 10 | 0.12 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 18 | 0.12 |
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 18 | 0.12 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 18 | 0.12 |
| (1,1219) | 1:111:A:TYR:H | 1:115:A:ILE:HB | 2 | 0.12 |
| (1,1218) | 1:111:A:TYR:H | 1:111:A:TYR:HB3 | 1 | 0.12 |
| (1,1216) | 1:110:A:GLY:HA2 | 1:111:A:TYR:H | 5 | 0.12 |
| (1,1204) | 1:100:A:ILE:HG21 | 1:106:A:TYR:H | 12 | 0.12 |
| (1,1204) | 1:100:A:ILE:HG22 | 1:106:A:TYR:H | 12 | 0.12 |
| (1,1204) | 1:100:A:ILE:HG23 | 1:106:A:TYR:H | 12 | 0.12 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 6 | 0.12 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 12 | 0.12 |
| (1,1172) | 1:102:A:TYR:H | 1:105:A:ALA:H | 19 | 0.12 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 8 | 0.12 |
| (1,1152) | 1:98:A:PHE:H | 1:123:A:PHE:HB3 | 13 | 0.12 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 13 | 0.12 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 6 | 0.12 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 6 | 0.12 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 6 | 0.12 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 12 | 0.12 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 12 | 0.12 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 12 | 0.12 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 17 | 0.12 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 17 | 0.12 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 17 | 0.12 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 10 | 0.12 |
| (1,1097) | 1:34:A:GLY:HA3 | 1:91:A:THR:H | 15 | 0.12 |
| (1,1092) | 1:90:A:MET:H | 1:90:A:MET:HG3 | 6 | 0.12 |
| (1,1065) | 1:79:A:VAL:HG21 | 1:85:A:GLN:H | 18 | 0.12 |
| (1,1065) | 1:79:A:VAL:HG22 | 1:85:A:GLN:H | 18 | 0.12 |
| (1,1065) | 1:79:A:VAL:HG23 | 1:85:A:GLN:H | 18 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1055) | 1:83:A:TRP:H | 1:85:A:GLN:H | 2 | 0.12 |
| (1,1037) | 1:80:A:ILE:HG12 | 1:83:A:TRP:H | 3 | 0.12 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG21 | 7 | 0.12 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG22 | 7 | 0.12 |
| (1,1030) | 1:82:A:GLY:H | 1:100:A:ILE:HG23 | 7 | 0.12 |
| (1,1001) | 1:73:A:THR:HB | 1:76:A:ALA:H | 7 | 0.12 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB1 | 18 | 0.12 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB2 | 18 | 0.12 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB3 | 18 | 0.12 |
| (1,966) | 1:69:A:PRO:HB3 | 1:70:A:PHE:H | 12 | 0.12 |
| (1,952) | 1:67:A:GLY:H | 1:68:A:LYS:HB2 | 6 | 0.12 |
| (1,919) | 1:60:A:PHE:HD1 | 1:61:A:ASP:H | 20 | 0.12 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 7 | 0.12 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 14 | 0.12 |
| (1,909) | 1:56:A:ASP:HA | 1:57:A:GLY:H | 17 | 0.12 |
| (1,897) | 1:59:A:GLN:HE21 | 1:62:A:SER:HB3 | 17 | 0.12 |
| (1,866) | 1:51:A:ASP:H | 1:124:A:GLU:HB3 | 5 | 0.12 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 1 | 0.12 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 6 | 0.12 |
| (1,830) | 1:46:A:VAL:H | 1:72:A:PHE:HA | 11 | 0.12 |
| (1,813) | 1:43:A:GLY:H | 1:74:A:LEU:HG | 19 | 0.12 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 14 | 0.12 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 19 | 0.12 |
| (1,797) | 1:41:A:GLN:H | 1:41:A:GLN:HG2 | 12 | 0.12 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG21 | 12 | 0.12 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG22 | 12 | 0.12 |
| (1,795) | 1:39:A:LYS:H | 1:130:A:VAL:HG23 | 12 | 0.12 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG21 | 1 | 0.12 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG22 | 1 | 0.12 |
| (1,789) | 1:38:A:THR:H | 1:91:A:THR:HG23 | 1 | 0.12 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 10 | 0.12 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 12 | 0.12 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 9 | 0.12 |
| (1,751) | 1:27:A:GLU:HG2 | 1:28:A:LYS:H | 10 | 0.12 |
| (1,748) | 1:27:A:GLU:H | 1:99:A:THR:HB | 1 | 0.12 |
| (1,748) | 1:27:A:GLU:H | 1:99:A:THR:HB | 15 | 0.12 |
| (1,697) | 1:79:A:VAL:HG11 | 1:83:A:TRP:HZ3 | 9 | 0.12 |
| (1,697) | 1:79:A:VAL:HG12 | 1:83:A:TRP:HZ3 | 9 | 0.12 |
| (1,697) | 1:79:A:VAL:HG13 | 1:83:A:TRP:HZ3 | 9 | 0.12 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG21 | 16 | 0.12 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG22 | 16 | 0.12 |
| (1,665) | 1:110:A:GLY:H | 1:115:A:ILE:HG23 | 16 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD11 | 10 | 0.12 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD12 | 10 | 0.12 |
| (1,637) | 1:46:A:VAL:HB | 1:127:A:LEU:HD13 | 10 | 0.12 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 1 | 0.12 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 1 | 0.12 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 1 | 0.12 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 13 | 0.12 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 13 | 0.12 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 13 | 0.12 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 18 | 0.12 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 18 | 0.12 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 18 | 0.12 |
| (1,546) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG2 | 3 | 0.12 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB1 | 14 | 0.12 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB2 | 14 | 0.12 |
| (1,495) | 1:102:A:TYR:HB2 | 1:105:A:ALA:HB3 | 14 | 0.12 |
| (1,481) | 1:100:A:ILE:HG21 | 1:104:A:LEU:HA | 10 | 0.12 |
| (1,481) | 1:100:A:ILE:HG22 | 1:104:A:LEU:HA | 10 | 0.12 |
| (1,481) | 1:100:A:ILE:HG23 | 1:104:A:LEU:HA | 10 | 0.12 |
| (1,470) | 1:100:A:ILE:HB | 1:121:A:LEU:HB2 | 16 | 0.12 |
| (1,460) | 1:97:A:LEU:HD11 | 1:98:A:PHE:H | 16 | 0.12 |
| (1,460) | 1:97:A:LEU:HD12 | 1:98:A:PHE:H | 16 | 0.12 |
| (1,460) | 1:97:A:LEU:HD13 | 1:98:A:PHE:H | 16 | 0.12 |
| (1,459) | 1:97:A:LEU:HG | 1:99:A:THR:H | 11 | 0.12 |
| (1,444) | 1:31:A:LEU:HG | 1:95:A:LYS:HB3 | 6 | 0.12 |
| (1,422) | 1:38:A:THR:HG21 | 1:91:A:THR:HA | 6 | 0.12 |
| (1,422) | 1:38:A:THR:HG22 | 1:91:A:THR:HA | 6 | 0.12 |
| (1,422) | 1:38:A:THR:HG23 | 1:91:A:THR:HA | 6 | 0.12 |
| (1,419) | 1:34:A:GLY:HA3 | 1:91:A:THR:HA | 1 | 0.12 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG21 | 6 | 0.12 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG22 | 6 | 0.12 |
| (1,405) | 1:85:A:GLN:HA | 1:89:A:THR:HG23 | 6 | 0.12 |
| (1,345) | 1:82:A:GLY:HA3 | 1:85:A:GLN:H | 6 | 0.12 |
| (1,328) | 1:80:A:ILE:HG13 | 1:83:A:TRP:H | 20 | 0.12 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG21 | 11 | 0.12 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG22 | 11 | 0.12 |
| (1,317) | 1:80:A:ILE:HB | 1:100:A:ILE:HG23 | 11 | 0.12 |
| (1,316) | 1:80:A:ILE:HB | 1:104:A:LEU:HB3 | 2 | 0.12 |
| (1,309) | 1:80:A:ILE:HA | 1:81:A:LYS:HB2 | 4 | 0.12 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG21 | 3 | 0.12 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG22 | 3 | 0.12 |
| (1,306) | 1:79:A:VAL:HB | 1:80:A:ILE:HG23 | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,289) | 1:76:A:ALA:HB1 | 1:78:A:GLU:HB2 | 13 | 0.12 |
| (1,289) | 1:76:A:ALA:HB2 | 1:78:A:GLU:HB2 | 13 | 0.12 |
| (1,289) | 1:76:A:ALA:HB3 | 1:78:A:GLU:HB2 | 13 | 0.12 |
| (1,227) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 6 | 0.12 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 6 | 0.12 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 12 | 0.12 |
| (1,220) | 1:66:A:ARG:HA | 1:66:A:ARG:HD2 | 4 | 0.12 |
| (1,192) | 1:59:A:GLN:HA | 1:61:A:ASP:H | 17 | 0.12 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG21 | 4 | 0.12 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG22 | 4 | 0.12 |
| (1,175) | 1:55:A:PRO:HG2 | 1:120:A:THR:HG23 | 4 | 0.12 |
| (1,149) | 1:50:A:TYR:HB2 | 1:123:A:PHE:HD2 | 15 | 0.12 |
| (1,130) | 1:48:A:VAL:HG11 | 1:50:A:TYR:HD1 | 9 | 0.12 |
| (1,130) | 1:48:A:VAL:HG12 | 1:50:A:TYR:HD1 | 9 | 0.12 |
| (1,130) | 1:48:A:VAL:HG13 | 1:50:A:TYR:HD1 | 9 | 0.12 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 10 | 0.12 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 10 | 0.12 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 10 | 0.12 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 11 | 0.12 |
| (1,109) | 1:46:A:VAL:HB | 1:129:A:ALA:H | 10 | 0.12 |
| (1,75) | 1:38:A:THR:HB | 1:40:A:PRO:HG3 | 6 | 0.12 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG21 | 15 | 0.12 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG22 | 15 | 0.12 |
| (1,49) | 1:35:A:ASP:HA | 1:37:A:VAL:HG23 | 15 | 0.12 |
| (1,26) | 1:27:A:GLU:HG3 | 1:99:A:THR:H | 9 | 0.12 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB1 | 17 | 0.12 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB2 | 17 | 0.12 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB3 | 17 | 0.12 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 7 | 0.12 |
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 13 | 0.11 |
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 13 | 0.11 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 13 | 0.11 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 13 | 0.11 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 13 | 0.11 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 13 | 0.11 |
| (1,1625) | 1:108:A:GLU:HG2 | 1:118:A:LYS:HG3 | 2 | 0.11 |
| (1,1625) | 1:108:A:GLU:HG3 | 1:118:A:LYS:HG3 | 2 | 0.11 |
| (1,1576) | 1:92:A:LEU:HD11 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1576) | 1:92:A:LEU:HD12 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1576) | 1:92:A:LEU:HD13 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1576) | 1:92:A:LEU:HD21 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1576) | 1:92:A:LEU:HD22 | 1:130:A:VAL:HB | 17 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1576) | 1:92:A:LEU:HD23 | 1:130:A:VAL:HB | 17 | 0.11 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB2 | 5 | 0.11 |
| (1,1528) | 1:82:A:GLY:HA3 | 1:85:A:GLN:HB3 | 5 | 0.11 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 20 | 0.11 |
| (1,1526) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 20 | 0.11 |
| (1,1523) | 1:78:A:GLU:HA | 1:78:A:GLU:HG2 | 10 | 0.11 |
| (1,1523) | 1:78:A:GLU:HA | 1:78:A:GLU:HG3 | 10 | 0.11 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 1 | 0.11 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 1 | 0.11 |
| (1,1506) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 14 | 0.11 |
| (1,1506) | 1:67:A:GLY:HA3 | 1:68:A:LYS:HB2 | 14 | 0.11 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD2 | 5 | 0.11 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD3 | 5 | 0.11 |
| (1,1483) | 1:62:A:SER:HB2 | 1:63:A:SER:H | 15 | 0.11 |
| (1,1483) | 1:62:A:SER:HB3 | 1:63:A:SER:H | 15 | 0.11 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 5 | 0.11 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 5 | 0.11 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE21 | 9 | 0.11 |
| (1,1471) | 1:59:A:GLN:H | 1:59:A:GLN:HE22 | 9 | 0.11 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG11 | 5 | 0.11 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG12 | 5 | 0.11 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG13 | 5 | 0.11 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG21 | 5 | 0.11 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG22 | 5 | 0.11 |
| (1,1454) | 1:54:A:PHE:HE1 | 1:114:A:VAL:HG23 | 5 | 0.11 |
| (1,1398) | 1:43:A:GLY:HA2 | 1:73:A:THR:HG21 | 4 | 0.11 |
| (1,1398) | 1:43:A:GLY:HA2 | 1:73:A:THR:HG22 | 4 | 0.11 |
| (1,1398) | 1:43:A:GLY:HA2 | 1:73:A:THR:HG23 | 4 | 0.11 |
| (1,1398) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 4 | 0.11 |
| (1,1398) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 4 | 0.11 |
| (1,1398) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 4 | 0.11 |
| (1,1367) | 1:35:A:ASP:HB2 | 1:37:A:VAL:HG21 | 8 | 0.11 |
| (1,1367) | 1:35:A:ASP:HB2 | 1:37:A:VAL:HG22 | 8 | 0.11 |
| (1,1367) | 1:35:A:ASP:HB2 | 1:37:A:VAL:HG23 | 8 | 0.11 |
| (1,1367) | 1:35:A:ASP:HB3 | 1:37:A:VAL:HG21 | 8 | 0.11 |
| (1,1367) | 1:35:A:ASP:HB3 | 1:37:A:VAL:HG22 | 8 | 0.11 |
| (1,1367) | 1:35:A:ASP:HB3 | 1:37:A:VAL:HG23 | 8 | 0.11 |
| (1,1324) | 1:19:A:PRO:HG2 | 1:55:A:PRO:HG2 | 1 | 0.11 |
| (1,1324) | 1:19:A:PRO:HG3 | 1:55:A:PRO:HG2 | 1 | 0.11 |
| (1,1317) | 1:13:A:GLU:HB2 | 1:14:A:ALA:H | 15 | 0.11 |
| (1,1317) | 1:13:A:GLU:HB3 | 1:14:A:ALA:H | 15 | 0.11 |
| (1,1309) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE22 | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1308) | 1:81:A:LYS:HD2 | 1:85:A:GLN:HE21 | 20 | 0.11 |
| (1,1305) | 1:71:A:GLN:HA | 1:71:A:GLN:HE22 | 20 | 0.11 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 5 | 0.11 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 5 | 0.11 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 5 | 0.11 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB1 | 17 | 0.11 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB2 | 17 | 0.11 |
| (1,1287) | 1:128:A:LEU:H | 1:129:A:ALA:HB3 | 17 | 0.11 |
| (1,1284) | 1:127:A:LEU:H | 1:127:A:LEU:HG | 7 | 0.11 |
| (1,1284) | 1:127:A:LEU:H | 1:127:A:LEU:HG | 17 | 0.11 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD21 | 14 | 0.11 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD22 | 14 | 0.11 |
| (1,1283) | 1:127:A:LEU:H | 1:127:A:LEU:HD23 | 14 | 0.11 |
| (1,1276) | 1:96:A:ALA:H | 1:127:A:LEU:H | 16 | 0.11 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG11 | 11 | 0.11 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG12 | 11 | 0.11 |
| (1,1259) | 1:124:A:GLU:H | 1:125:A:VAL:HG13 | 11 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 10 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 10 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 10 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 12 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 12 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 12 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB1 | 1:120:A:THR:H | 16 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB2 | 1:120:A:THR:H | 16 | 0.11 |
| (1,1236) | 1:119:A:ALA:HB3 | 1:120:A:THR:H | 16 | 0.11 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 3 | 0.11 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 14 | 0.11 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 17 | 0.11 |
| (1,1184) | 1:103:A:GLN:H | 1:104:A:LEU:HB2 | 15 | 0.11 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 5 | 0.11 |
| (1,1147) | 1:98:A:PHE:H | 1:99:A:THR:H | 6 | 0.11 |
| (1,1113) | 1:91:A:THR:HG21 | 1:92:A:LEU:H | 10 | 0.11 |
| (1,1113) | 1:91:A:THR:HG22 | 1:92:A:LEU:H | 10 | 0.11 |
| (1,1113) | 1:91:A:THR:HG23 | 1:92:A:LEU:H | 10 | 0.11 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 19 | 0.11 |
| (1,1105) | 1:38:A:THR:H | 1:92:A:LEU:H | 8 | 0.11 |
| (1,1104) | 1:91:A:THR:H | 1:127:A:LEU:HG | 14 | 0.11 |
| (1,1065) | 1:79:A:VAL:HG21 | 1:85:A:GLN:H | 20 | 0.11 |
| (1,1065) | 1:79:A:VAL:HG22 | 1:85:A:GLN:H | 20 | 0.11 |
| (1,1065) | 1:79:A:VAL:HG23 | 1:85:A:GLN:H | 20 | 0.11 |
| (1,1009) | 1:76:A:ALA:H | 1:78:A:GLU:H | 4 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG21 | 12 | 0.11 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG22 | 12 | 0.11 |
| (1,1008) | 1:77:A:GLY:H | 1:79:A:VAL:HG23 | 12 | 0.11 |
| (1,1003) | 1:74:A:LEU:HB3 | 1:76:A:ALA:H | 20 | 0.11 |
| (1,977) | 1:47:A:THR:HG21 | 1:71:A:GLN:H | 3 | 0.11 |
| (1,977) | 1:47:A:THR:HG22 | 1:71:A:GLN:H | 3 | 0.11 |
| (1,977) | 1:47:A:THR:HG23 | 1:71:A:GLN:H | 3 | 0.11 |
| (1,910) | 1:55:A:PRO:HA | 1:57:A:GLY:H | 20 | 0.11 |
| (1,887) | 1:53:A:ARG:HB3 | 1:54:A:PHE:H | 2 | 0.11 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG11 | 2 | 0.11 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG12 | 2 | 0.11 |
| (1,868) | 1:51:A:ASP:H | 1:125:A:VAL:HG13 | 2 | 0.11 |
| (1,863) | 1:50:A:TYR:HB2 | 1:51:A:ASP:H | 19 | 0.11 |
| (1,837) | 1:47:A:THR:H | 1:71:A:GLN:HA | 15 | 0.11 |
| (1,836) | 1:47:A:THR:H | 1:128:A:LEU:H | 2 | 0.11 |
| (1,828) | 1:46:A:VAL:H | 1:71:A:GLN:HA | 1 | 0.11 |
| (1,787) | 1:37:A:VAL:HB | 1:38:A:THR:H | 16 | 0.11 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG21 | 10 | 0.11 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG22 | 10 | 0.11 |
| (1,783) | 1:37:A:VAL:H | 1:91:A:THR:HG23 | 10 | 0.11 |
| (1,744) | 1:26:A:LEU:H | 1:27:A:GLU:HG3 | 7 | 0.11 |
| (1,684) | 1:48:A:VAL:HG21 | 1:50:A:TYR:HE1 | 10 | 0.11 |
| (1,684) | 1:48:A:VAL:HG22 | 1:50:A:TYR:HE1 | 10 | 0.11 |
| (1,684) | 1:48:A:VAL:HG23 | 1:50:A:TYR:HE1 | 10 | 0.11 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG21 | 6 | 0.11 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG22 | 6 | 0.11 |
| (1,657) | 1:38:A:THR:HB | 1:130:A:VAL:HG23 | 6 | 0.11 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG11 | 11 | 0.11 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG12 | 11 | 0.11 |
| (1,656) | 1:38:A:THR:HB | 1:130:A:VAL:HG13 | 11 | 0.11 |
| (1,581) | 1:55:A:PRO:HG3 | 1:120:A:THR:HB | 2 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 7 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 7 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 7 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 9 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 9 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 9 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 11 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 11 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 11 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 14 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 14 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 14 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG21 | 20 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG22 | 20 | 0.11 |
| (1,562) | 1:114:A:VAL:HA | 1:114:A:VAL:HG23 | 20 | 0.11 |
| (1,536) | 1:102:A:TYR:HE2 | 1:108:A:GLU:HB2 | 19 | 0.11 |
| (1,498) | 1:103:A:GLN:HA | 1:104:A:LEU:HG | 1 | 0.11 |
| (1,498) | 1:103:A:GLN:HA | 1:104:A:LEU:HG | 2 | 0.11 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB1 | 14 | 0.11 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB2 | 14 | 0.11 |
| (1,487) | 1:102:A:TYR:HA | 1:105:A:ALA:HB3 | 14 | 0.11 |
| (1,425) | 1:92:A:LEU:HG | 1:93:A:GLY:H | 14 | 0.11 |
| (1,413) | 1:90:A:MET:HE1 | 1:91:A:THR:H | 5 | 0.11 |
| (1,413) | 1:90:A:MET:HE2 | 1:91:A:THR:H | 5 | 0.11 |
| (1,413) | 1:90:A:MET:HE3 | 1:91:A:THR:H | 5 | 0.11 |
| (1,378) | 1:81:A:LYS:HA | 1:84:A:ASP:HB3 | 16 | 0.11 |
| (1,355) | 1:81:A:LYS:HB3 | 1:82:A:GLY:HA2 | 17 | 0.11 |
| (1,347) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HB2 | 4 | 0.11 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD21 | 18 | 0.11 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD22 | 18 | 0.11 |
| (1,341) | 1:81:A:LYS:HG3 | 1:104:A:LEU:HD23 | 18 | 0.11 |
| (1,328) | 1:80:A:ILE:HG13 | 1:83:A:TRP:H | 12 | 0.11 |
| (1,294) | 1:78:A:GLU:H | 1:78:A:GLU:HG2 | 15 | 0.11 |
| (1,276) | 1:74:A:LEU:HD11 | 1:88:A:ALA:H | 14 | 0.11 |
| (1,276) | 1:74:A:LEU:HD12 | 1:88:A:ALA:H | 14 | 0.11 |
| (1,276) | 1:74:A:LEU:HD13 | 1:88:A:ALA:H | 14 | 0.11 |
| (1,274) | 1:74:A:LEU:HD11 | 1:87:A:VAL:H | 19 | 0.11 |
| (1,274) | 1:74:A:LEU:HD12 | 1:87:A:VAL:H | 19 | 0.11 |
| (1,274) | 1:74:A:LEU:HD13 | 1:87:A:VAL:H | 19 | 0.11 |
| (1,266) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 11 | 0.11 |
| (1,266) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 11 | 0.11 |
| (1,266) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 11 | 0.11 |
| (1,224) | 1:67:A:GLY:HA2 | 1:68:A:LYS:HB2 | 4 | 0.11 |
| (1,220) | 1:66:A:ARG:HA | 1:66:A:ARG:HD2 | 8 | 0.11 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 17 | 0.11 |
| (1,198) | 1:59:A:GLN:HG2 | 1:61:A:ASP:H | 10 | 0.11 |
| (1,169) | 1:53:A:ARG:HD2 | 1:59:A:GLN:H | 16 | 0.11 |
| (1,161) | 1:53:A:ARG:HA | 1:60:A:PHE:H | 8 | 0.11 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 2 | 0.11 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 2 | 0.11 |
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 2 | 0.11 |
| (1,129) | 1:48:A:VAL:HG11 | 1:128:A:LEU:H | 15 | 0.11 |
| (1,129) | 1:48:A:VAL:HG12 | 1:128:A:LEU:H | 15 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,129) | 1:48:A:VAL:HG13 | 1:128:A:LEU:H | 15 | 0.11 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 15 | 0.11 |
| (1,123) | 1:46:A:VAL:HG11 | 1:130:A:VAL:HB | 8 | 0.11 |
| (1,123) | 1:46:A:VAL:HG12 | 1:130:A:VAL:HB | 8 | 0.11 |
| (1,123) | 1:46:A:VAL:HG13 | 1:130:A:VAL:HB | 8 | 0.11 |
| (1,114) | 1:46:A:VAL:HG21 | 1:47:A:THR:H | 8 | 0.11 |
| (1,114) | 1:46:A:VAL:HG22 | 1:47:A:THR:H | 8 | 0.11 |
| (1,114) | 1:46:A:VAL:HG23 | 1:47:A:THR:H | 8 | 0.11 |
| (1,109) | 1:46:A:VAL:HB | 1:129:A:ALA:H | 9 | 0.11 |
| (1,100) | 1:45:A:LYS:HB3 | 1:46:A:VAL:HA | 14 | 0.11 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 11 | 0.11 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 12 | 0.11 |
| (1,98) | 1:45:A:LYS:HB3 | 1:46:A:VAL:H | 15 | 0.11 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG21 | 2 | 0.11 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG22 | 2 | 0.11 |
| (1,78) | 1:40:A:PRO:HD3 | 1:91:A:THR:HG23 | 2 | 0.11 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG21 | 16 | 0.11 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG22 | 16 | 0.11 |
| (1,73) | 1:40:A:PRO:HB3 | 1:46:A:VAL:HG23 | 16 | 0.11 |
| (1,68) | 1:38:A:THR:HG21 | 1:92:A:LEU:HA | 20 | 0.11 |
| (1,68) | 1:38:A:THR:HG22 | 1:92:A:LEU:HA | 20 | 0.11 |
| (1,68) | 1:38:A:THR:HG23 | 1:92:A:LEU:HA | 20 | 0.11 |
| (1,45) | 1:34:A:GLY:HA3 | 1:94:A:GLU:HB2 | 12 | 0.11 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB1 | 5 | 0.11 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB2 | 5 | 0.11 |
| (1,17) | 1:41:A:GLN:HA | 1:42:A:ALA:HB3 | 5 | 0.11 |
| (1,1647) | 1:121:A:LEU:HD11 | 1:122:A:VAL:H | 7 | 0.1 |
| (1,1647) | 1:121:A:LEU:HD12 | 1:122:A:VAL:H | 7 | 0.1 |
| (1,1647) | 1:121:A:LEU:HD13 | 1:122:A:VAL:H | 7 | 0.1 |
| (1,1647) | 1:121:A:LEU:HD21 | 1:122:A:VAL:H | 7 | 0.1 |
| (1,1647) | 1:121:A:LEU:HD22 | 1:122:A:VAL:H | 7 | 0.1 |
| (1,1647) | 1:121:A:LEU:HD23 | 1:122:A:VAL:H | 7 | 0.1 |
| (1,1596) | 1:97:A:LEU:HD11 | 1:124:A:GLU:H | 10 | 0.1 |
| (1,1596) | 1:97:A:LEU:HD12 | 1:124:A:GLU:H | 10 | 0.1 |
| (1,1596) | 1:97:A:LEU:HD13 | 1:124:A:GLU:H | 10 | 0.1 |
| (1,1596) | 1:97:A:LEU:HD21 | 1:124:A:GLU:H | 10 | 0.1 |
| (1,1596) | 1:97:A:LEU:HD22 | 1:124:A:GLU:H | 10 | 0.1 |
| (1,1596) | 1:97:A:LEU:HD23 | 1:124:A:GLU:H | 10 | 0.1 |
| (1,1594) | 1:97:A:LEU:HD11 | 1:123:A:PHE:H | 20 | 0.1 |
| (1,1594) | 1:97:A:LEU:HD12 | 1:123:A:PHE:H | 20 | 0.1 |
| (1,1594) | 1:97:A:LEU:HD13 | 1:123:A:PHE:H | 20 | 0.1 |
| (1,1594) | 1:97:A:LEU:HD21 | 1:123:A:PHE:H | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1594) | 1:97:A:LEU:HD22 | 1:123:A:PHE:H | 20 | 0.1 |
| (1,1594) | 1:97:A:LEU:HD23 | 1:123:A:PHE:H | 20 | 0.1 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB2 | 13 | 0.1 |
| (1,1532) | 1:84:A:ASP:HB2 | 1:85:A:GLN:HB3 | 13 | 0.1 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB1 | 4 | 0.1 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB2 | 4 | 0.1 |
| (1,1519) | 1:71:A:GLN:HG2 | 1:129:A:ALA:HB3 | 4 | 0.1 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB1 | 4 | 0.1 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB2 | 4 | 0.1 |
| (1,1519) | 1:71:A:GLN:HG3 | 1:129:A:ALA:HB3 | 4 | 0.1 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD2 | 3 | 0.1 |
| (1,1491) | 1:64:A:ARG:HA | 1:64:A:ARG:HD3 | 3 | 0.1 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD2 | 20 | 0.1 |
| (1,1490) | 1:64:A:ARG:H | 1:64:A:ARG:HD3 | 20 | 0.1 |
| (1,1433) | 1:51:A:ASP:HB2 | 1:124:A:GLU:HB3 | 12 | 0.1 |
| (1,1433) | 1:51:A:ASP:HB3 | 1:124:A:GLU:HB3 | 12 | 0.1 |
| (1,1346) | 1:28:A:LYS:HG2 | 1:30:A:VAL:H | 9 | 0.1 |
| (1,1346) | 1:28:A:LYS:HG3 | 1:30:A:VAL:H | 9 | 0.1 |
| (1,1193) | 1:105:A:ALA:H | 1:107:A:GLY:H | 12 | 0.1 |
| (1,1126) | 1:94:A:GLU:H | 1:127:A:LEU:HG | 13 | 0.1 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 12 | 0.1 |
| (1,1106) | 1:37:A:VAL:H | 1:92:A:LEU:H | 14 | 0.1 |
| (1,1105) | 1:38:A:THR:H | 1:92:A:LEU:H | 12 | 0.1 |
| (1,1065) | 1:79:A:VAL:HG21 | 1:85:A:GLN:H | 9 | 0.1 |
| (1,1065) | 1:79:A:VAL:HG22 | 1:85:A:GLN:H | 9 | 0.1 |
| (1,1065) | 1:79:A:VAL:HG23 | 1:85:A:GLN:H | 9 | 0.1 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB1 | 7 | 0.1 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB2 | 7 | 0.1 |
| (1,984) | 1:73:A:THR:H | 1:76:A:ALA:HB3 | 7 | 0.1 |
| (1,938) | 1:64:A:ARG:H | 1:64:A:ARG:HG3 | 14 | 0.1 |
| (1,930) | 1:63:A:SER:H | 1:64:A:ARG:HB3 | 16 | 0.1 |
| (1,913) | 1:53:A:ARG:HB3 | 1:57:A:GLY:H | 15 | 0.1 |
| (1,901) | 1:59:A:GLN:HG2 | 1:59:A:GLN:HE22 | 19 | 0.1 |
| (1,866) | 1:51:A:ASP:H | 1:124:A:GLU:HB3 | 17 | 0.1 |
| (1,836) | 1:47:A:THR:H | 1:128:A:LEU:H | 1 | 0.1 |
| (1,812) | 1:43:A:GLY:H | 1:44:A:LYS:HB2 | 20 | 0.1 |
| (1,807) | 1:42:A:ALA:H | 1:43:A:GLY:H | 17 | 0.1 |
| (1,806) | 1:42:A:ALA:H | 1:74:A:LEU:HG | 16 | 0.1 |
| (1,781) | 1:37:A:VAL:H | 1:91:A:THR:HB | 11 | 0.1 |
| (1,776) | 1:33:A:PRO:HB2 | 1:34:A:GLY:H | 17 | 0.1 |
| (1,686) | 1:102:A:TYR:HE2 | 1:118:A:LYS:HA | 14 | 0.1 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB1 | 15 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB2 | 15 | 0.1 |
| (1,638) | 1:127:A:LEU:HD11 | 1:129:A:ALA:HB3 | 15 | 0.1 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB1 | 15 | 0.1 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB2 | 15 | 0.1 |
| (1,638) | 1:127:A:LEU:HD12 | 1:129:A:ALA:HB3 | 15 | 0.1 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB1 | 15 | 0.1 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB2 | 15 | 0.1 |
| (1,638) | 1:127:A:LEU:HD13 | 1:129:A:ALA:HB3 | 15 | 0.1 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD11 | 6 | 0.1 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD12 | 6 | 0.1 |
| (1,634) | 1:47:A:THR:H | 1:127:A:LEU:HD13 | 6 | 0.1 |
| (1,603) | 1:123:A:PHE:H | 1:124:A:GLU:HA | 4 | 0.1 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG21 | 4 | 0.1 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG22 | 4 | 0.1 |
| (1,584) | 1:55:A:PRO:HG3 | 1:120:A:THR:HG23 | 4 | 0.1 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 4 | 0.1 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 4 | 0.1 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 4 | 0.1 |
| (1,578) | 1:119:A:ALA:HB1 | 1:120:A:THR:HB | 20 | 0.1 |
| (1,578) | 1:119:A:ALA:HB2 | 1:120:A:THR:HB | 20 | 0.1 |
| (1,578) | 1:119:A:ALA:HB3 | 1:120:A:THR:HB | 20 | 0.1 |
| (1,543) | 1:108:A:GLU:HA | 1:118:A:LYS:HG2 | 2 | 0.1 |
| (1,521) | 1:80:A:ILE:HD11 | 1:105:A:ALA:HA | 8 | 0.1 |
| (1,521) | 1:80:A:ILE:HD12 | 1:105:A:ALA:HA | 8 | 0.1 |
| (1,521) | 1:80:A:ILE:HD13 | 1:105:A:ALA:HA | 8 | 0.1 |
| (1,520) | 1:100:A:ILE:HG21 | 1:105:A:ALA:HA | 2 | 0.1 |
| (1,520) | 1:100:A:ILE:HG22 | 1:105:A:ALA:HA | 2 | 0.1 |
| (1,520) | 1:100:A:ILE:HG23 | 1:105:A:ALA:HA | 2 | 0.1 |
| (1,518) | 1:80:A:ILE:HA | 1:105:A:ALA:HA | 19 | 0.1 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD11 | 18 | 0.1 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD12 | 18 | 0.1 |
| (1,350) | 1:82:A:GLY:HA3 | 1:104:A:LEU:HD13 | 18 | 0.1 |
| (1,330) | 1:79:A:VAL:HG21 | 1:83:A:TRP:HE3 | 9 | 0.1 |
| (1,330) | 1:79:A:VAL:HG22 | 1:83:A:TRP:HE3 | 9 | 0.1 |
| (1,330) | 1:79:A:VAL:HG23 | 1:83:A:TRP:HE3 | 9 | 0.1 |
| (1,278) | 1:74:A:LEU:HD11 | 1:87:A:VAL:HB | 14 | 0.1 |
| (1,278) | 1:74:A:LEU:HD12 | 1:87:A:VAL:HB | 14 | 0.1 |
| (1,278) | 1:74:A:LEU:HD13 | 1:87:A:VAL:HB | 14 | 0.1 |
| (1,208) | 1:63:A:SER:H | 1:64:A:ARG:HA | 3 | 0.1 |
| (1,191) | 1:54:A:PHE:HD1 | 1:58:A:LYS:HD3 | 14 | 0.1 |
| (1,127) | 1:47:A:THR:HB | 1:48:A:VAL:HA | 8 | 0.1 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG21 | 19 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|-----------------|-----------------|----------|---------------|
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG22 | 19 | 0.1 |
| (1,90) | 1:43:A:GLY:HA3 | 1:73:A:THR:HG23 | 19 | 0.1 |
| (1,64) | 1:38:A:THR:HG21 | 1:39:A:LYS:H | 13 | 0.1 |
| (1,64) | 1:38:A:THR:HG22 | 1:39:A:LYS:H | 13 | 0.1 |
| (1,64) | 1:38:A:THR:HG23 | 1:39:A:LYS:H | 13 | 0.1 |
| (1,48) | 1:34:A:GLY:HA2 | 1:94:A:GLU:HB3 | 15 | 0.1 |
| (1,45) | 1:34:A:GLY:HA3 | 1:94:A:GLU:HB2 | 18 | 0.1 |
| (1,16) | 1:41:A:GLN:H | 1:41:A:GLN:HB2 | 11 | 0.1 |

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

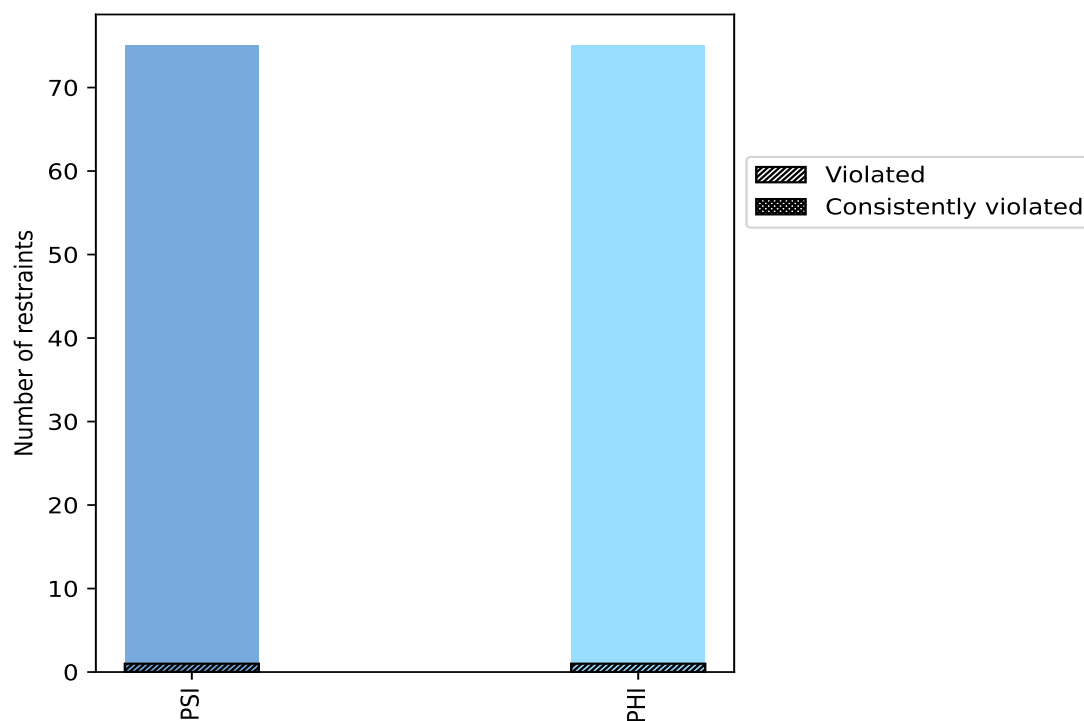
10.1 Summary of dihedral-angle violations [i](#)

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

| Angle type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| PSI | 75 | 50.0 | 1 | 1.3 | 0.7 | 0 | 0.0 | 0.0 |
| PHI | 75 | 50.0 | 1 | 1.3 | 0.7 | 0 | 0.0 | 0.0 |
| Total | 150 | 100.0 | 2 | 1.3 | 1.3 | 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](#)



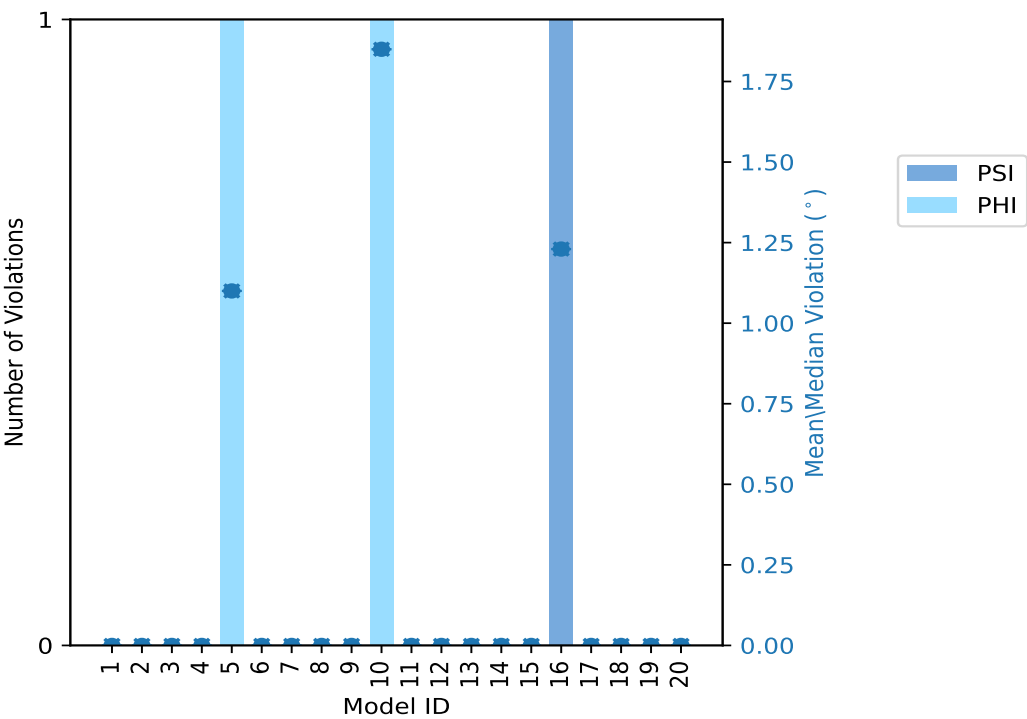
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PSI | PHI | Total | | | | |
| 1 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 2 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 3 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 4 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 5 | 0 | 1 | 1 | 1.1 | 1.1 | 0.0 | 1.1 |
| 6 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 7 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 8 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 9 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 10 | 0 | 1 | 1 | 1.85 | 1.85 | 0.0 | 1.85 |
| 11 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 12 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 13 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 14 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 15 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 16 | 1 | 0 | 1 | 1.23 | 1.23 | 0.0 | 1.23 |
| 17 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 18 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 19 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 20 | 0 | 0 | 0 | 0.0 | 0.0 | 0.0 | 0.0 |

10.2.1 Bar graph : Dihedral 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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

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

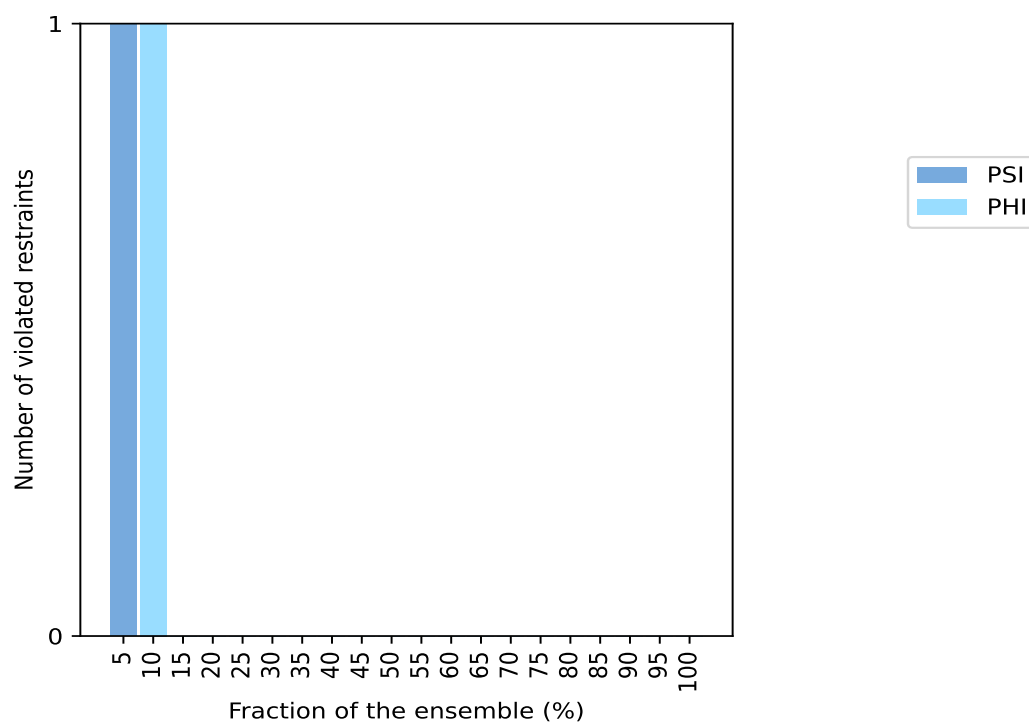
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 0 | 0 |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

¹ Number of models with violations

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

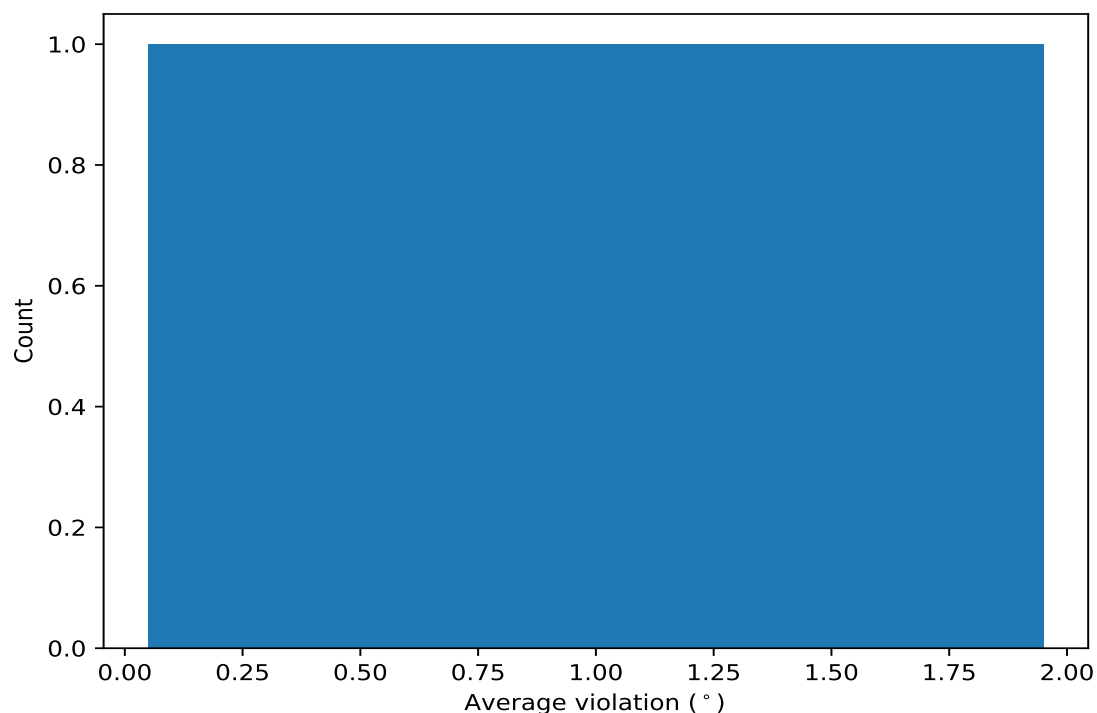


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|--------|--------------|--------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,39) | 1:50:A:TYR:C | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C | 2 | 1.48 | 0.38 | 1.48 |

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.

Data insufficient to plot histogram

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 (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,39) | 1:50:A:TYR:C | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C | 10 | 1.85 |
| (1,54) | 1:64:A:ARG:N | 1:64:A:ARG:CA | 1:64:A:ARG:C | 1:65:A:SER:N | 16 | 1.23 |
| (1,39) | 1:50:A:TYR:C | 1:51:A:ASP:N | 1:51:A:ASP:CA | 1:51:A:ASP:C | 5 | 1.1 |