



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 10:03 PM EST

PDB ID : 2MIU
BMRB ID : 19694
Title : Structure of FHL2 LIM adaptor and its Interaction with Ski
Authors : Yang, Y.; Sun, Y.; Medrano, E.E.; Tian, X.; Weiss, M.A.
Deposited on : 2013-12-20

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

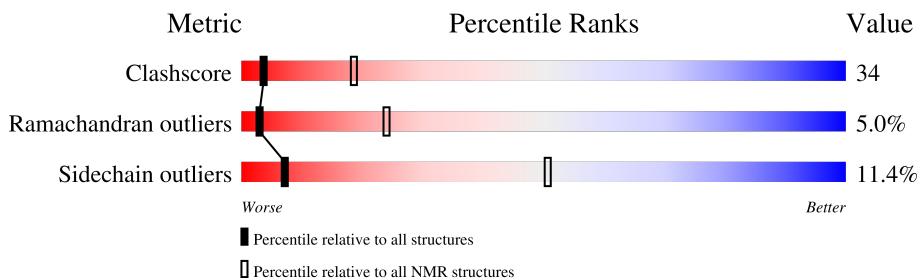
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 79%.

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 | 98 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:5-A:98 (94) | 0.54 | 9 |

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

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

The models can be grouped into 5 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1518 atoms, of which 719 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Four and a half LIM domains protein 2.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|----|-------|
| 1 | A | 98 | Total | C | H | N | O | S | 0 |
| | | | 1515 | 493 | 719 | 134 | 155 | 14 | |

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

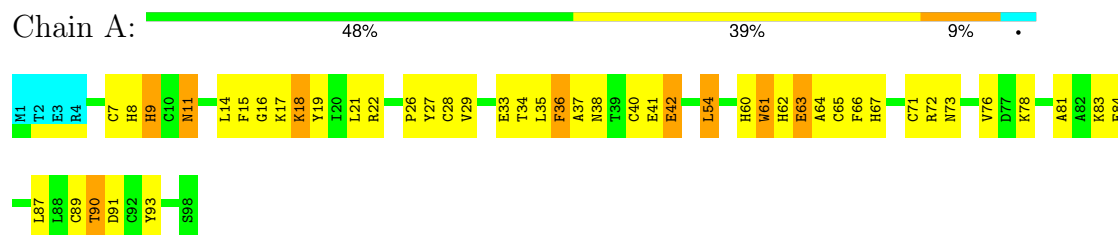
| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| 2 | A | 3 | Total | Zn |
| | | | 3 | 3 |

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: Four and a half LIM domains protein 2

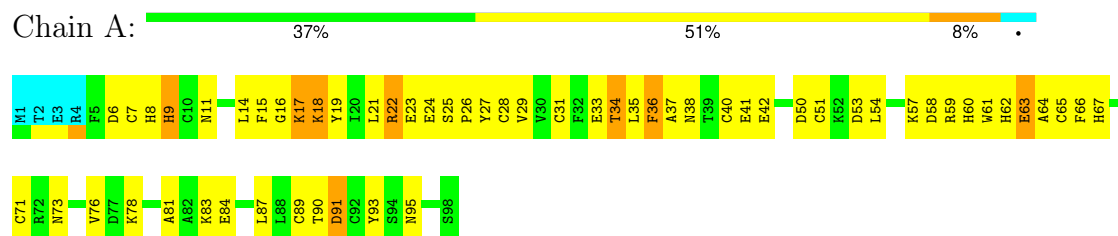


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

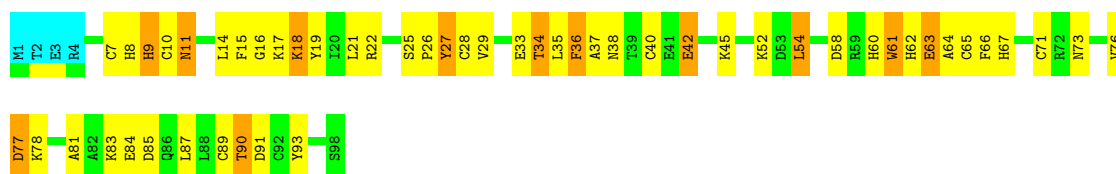
- Molecule 1: Four and a half LIM domains protein 2



4.2.2 Score per residue for model 2

- Molecule 1: Four and a half LIM domains protein 2

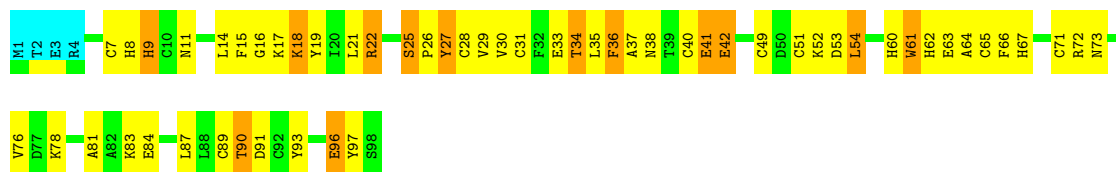




4.2.3 Score per residue for model 3

- Molecule 1: Four and a half LIM domains protein 2

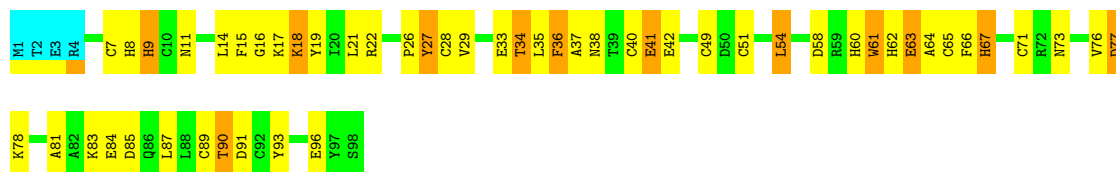
Chain A: 39% 44% 13% .



4.2.4 Score per residue for model 4

- Molecule 1: Four and a half LIM domains protein 2

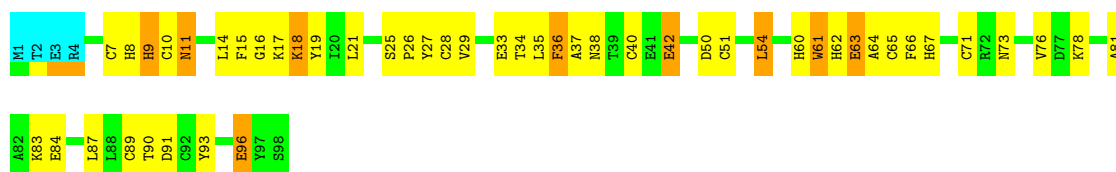
Chain A: 43% 41% 12% .



4.2.5 Score per residue for model 5

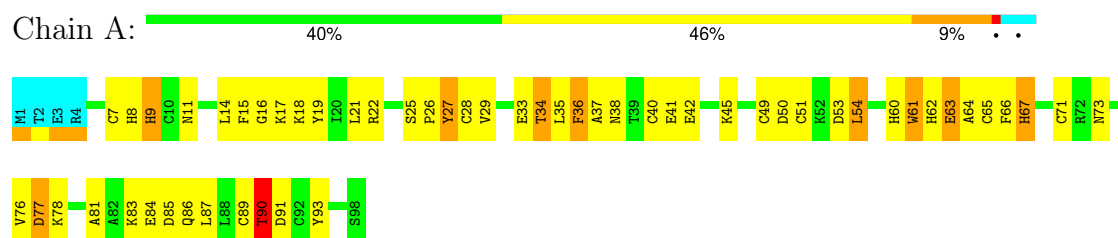
- Molecule 1: Four and a half LIM domains protein 2

Chain A: 46% 41% 9% .



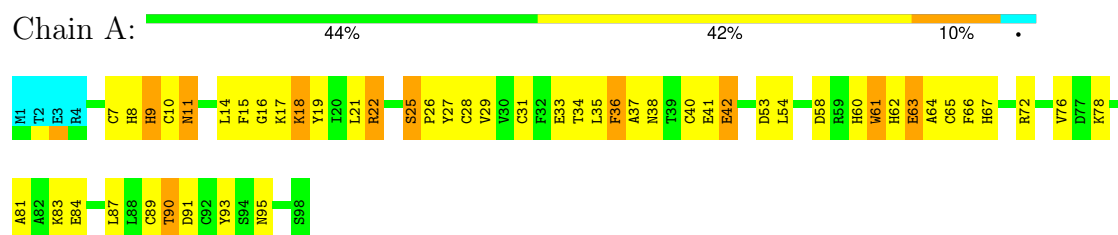
4.2.6 Score per residue for model 6

- Molecule 1: Four and a half LIM domains protein 2



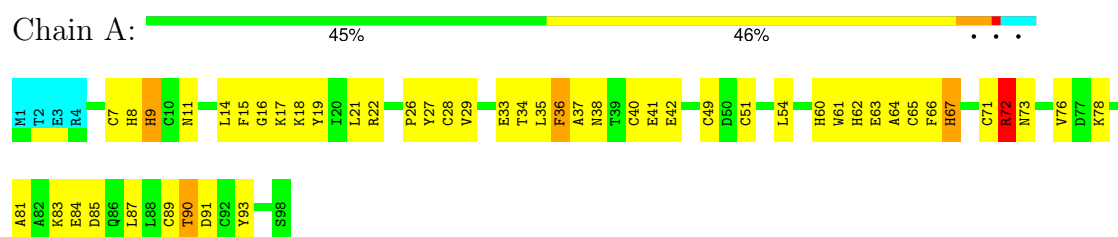
4.2.7 Score per residue for model 7

- Molecule 1: Four and a half LIM domains protein 2



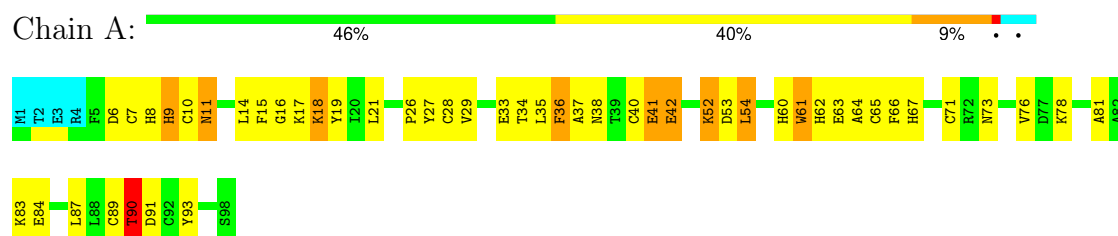
4.2.8 Score per residue for model 8

- Molecule 1: Four and a half LIM domains protein 2



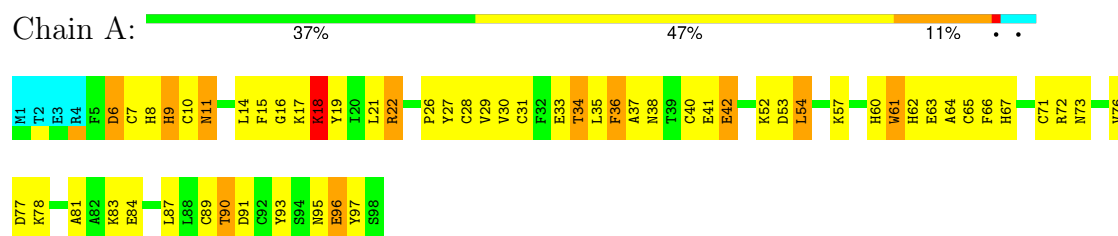
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Four and a half LIM domains protein 2



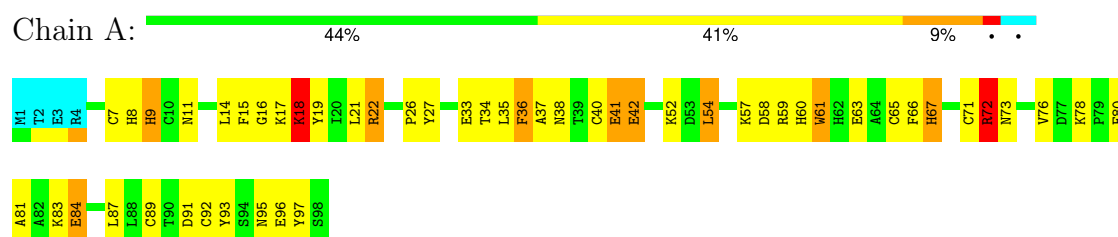
4.2.10 Score per residue for model 10

- Molecule 1: Four and a half LIM domains protein 2



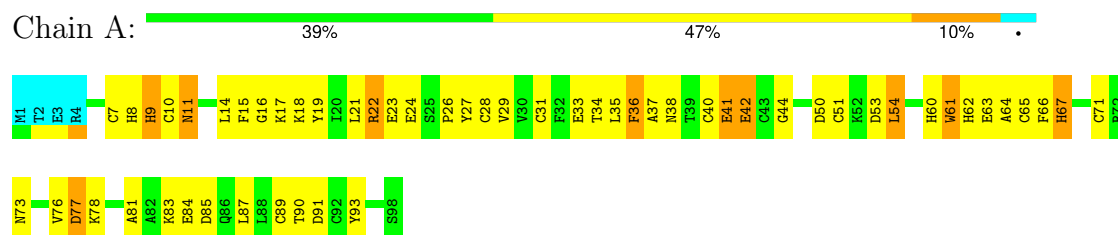
4.2.11 Score per residue for model 11

- Molecule 1: Four and a half LIM domains protein 2



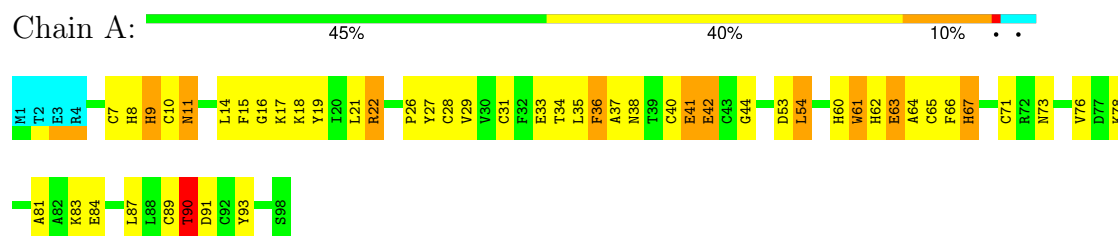
4.2.12 Score per residue for model 12

- Molecule 1: Four and a half LIM domains protein 2



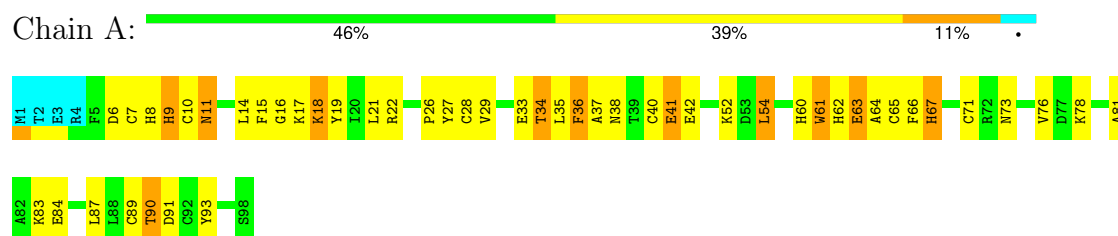
4.2.13 Score per residue for model 13

- Molecule 1: Four and a half LIM domains protein 2



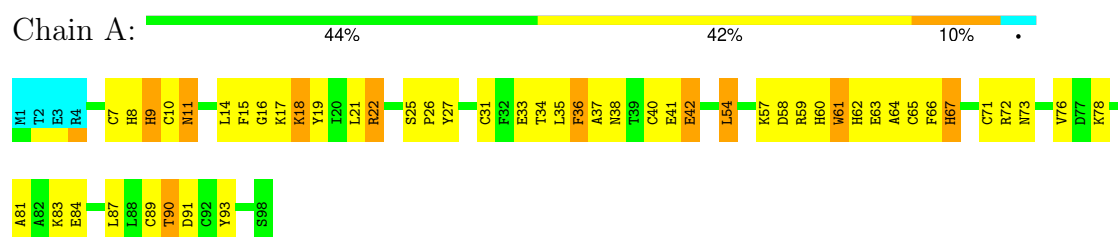
4.2.14 Score per residue for model 14

- Molecule 1: Four and a half LIM domains protein 2



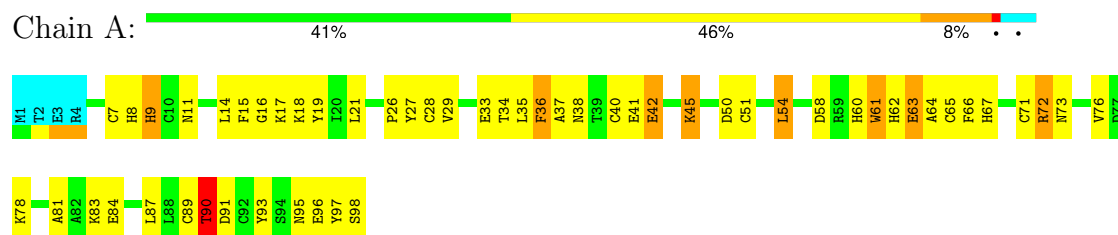
4.2.15 Score per residue for model 15

- Molecule 1: Four and a half LIM domains protein 2



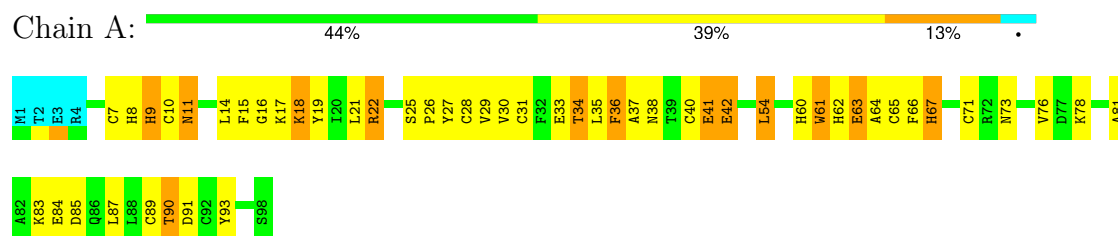
4.2.16 Score per residue for model 16

- Molecule 1: Four and a half LIM domains protein 2



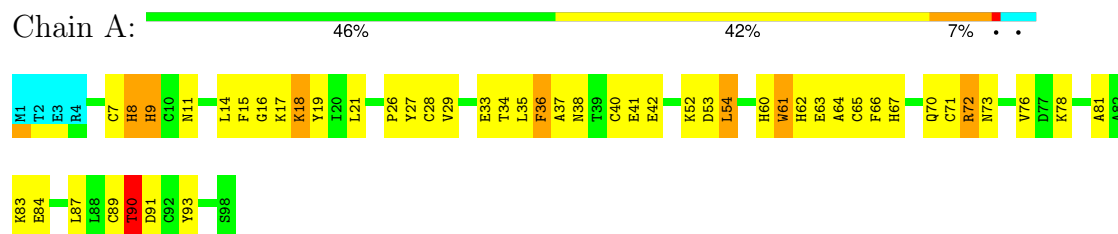
4.2.17 Score per residue for model 17

- Molecule 1: Four and a half LIM domains protein 2



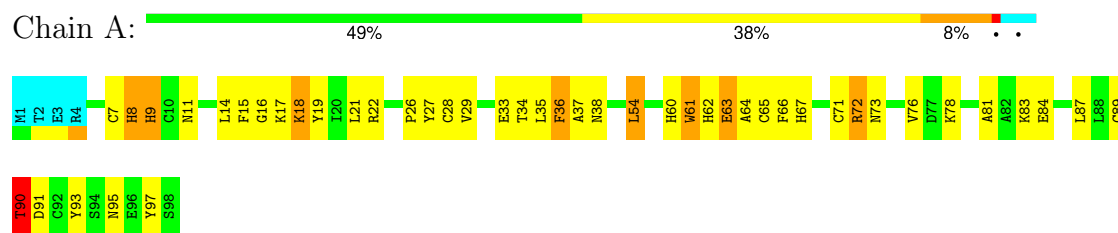
4.2.18 Score per residue for model 18

- Molecule 1: Four and a half LIM domains protein 2



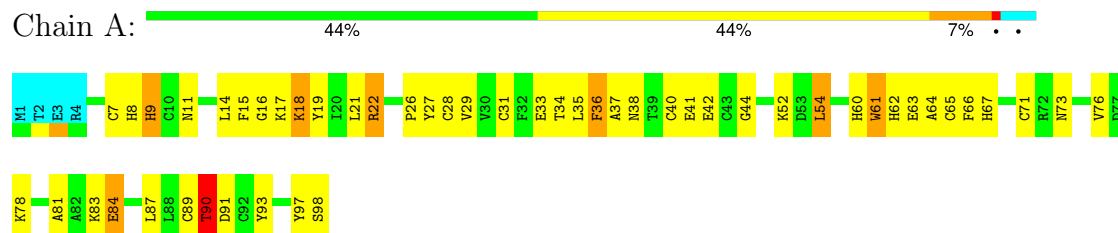
4.2.19 Score per residue for model 19

- Molecule 1: Four and a half LIM domains protein 2



4.2.20 Score per residue for model 20

- Molecule 1: Four and a half LIM domains protein 2



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| X-PLOR NIH | structure solution | |
| X-PLOR NIH | refinement | |

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

| | |
|--|----------------|
| Chemical shift file(s) | working_cs.cif |
| Number of chemical shift lists | 1 |
| Total number of shifts | 1010 |
| Number of shifts mapped to atoms | 1010 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 79% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------------|-------------|-----------------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.08±0.00 | 0±0/781 (0.0± 0.0%) | 0.92±0.00 | 1±0/1051 (0.1± 0.0%) |
| All | All | 1.08 | 0/15620 (0.0%) | 0.92 | 20/21020 (0.1%) |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) | Models | |
|-----|-------|-----|------|-----------|-------|-------------|----------|--------|-------|
| | | | | | | | | Worst | Total |
| 1 | A | 27 | TYR | CB-CG-CD2 | -5.94 | 117.44 | 121.00 | 12 | 20 |

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 761 | 682 | 682 | 50±4 |
| All | All | 15280 | 13640 | 13640 | 992 |

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 34.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:21:LEU:HD22 | 1:A:21:LEU:N | 0.64 | 2.07 | 12 | 20 |
| 1:A:38:ASN:ND2 | 1:A:60:HIS:NE2 | 0.62 | 2.47 | 19 | 11 |
| 1:A:67:HIS:ND1 | 1:A:67:HIS:N | 0.62 | 2.48 | 17 | 9 |
| 1:A:8:HIS:N | 1:A:26:PRO:O | 0.60 | 2.35 | 3 | 20 |
| 1:A:14:LEU:HD22 | 1:A:14:LEU:N | 0.60 | 2.12 | 8 | 20 |
| 1:A:38:ASN:ND2 | 1:A:60:HIS:CE1 | 0.59 | 2.70 | 3 | 7 |
| 1:A:38:ASN:ND2 | 1:A:60:HIS:CD2 | 0.59 | 2.71 | 15 | 10 |
| 1:A:15:PHE:O | 1:A:15:PHE:CD2 | 0.58 | 2.56 | 14 | 20 |
| 1:A:36:PHE:CD1 | 1:A:36:PHE:N | 0.58 | 2.71 | 19 | 20 |
| 1:A:71:CYS:O | 1:A:73:ASN:N | 0.58 | 2.37 | 8 | 17 |
| 1:A:33:GLU:O | 1:A:37:ALA:HB2 | 0.57 | 1.99 | 2 | 20 |
| 1:A:33:GLU:O | 1:A:37:ALA:N | 0.57 | 2.37 | 1 | 20 |
| 1:A:21:LEU:N | 1:A:21:LEU:CD2 | 0.56 | 2.69 | 8 | 20 |
| 1:A:22:ARG:CG | 1:A:22:ARG:HH11 | 0.55 | 2.13 | 1 | 10 |
| 1:A:7:CYS:O | 1:A:11:ASN:N | 0.55 | 2.38 | 3 | 20 |
| 1:A:22:ARG:CG | 1:A:22:ARG:NH1 | 0.55 | 2.70 | 1 | 10 |
| 1:A:38:ASN:OD1 | 1:A:60:HIS:NE2 | 0.54 | 2.41 | 8 | 5 |
| 1:A:89:CYS:O | 1:A:91:ASP:N | 0.54 | 2.41 | 13 | 20 |
| 1:A:11:ASN:O | 1:A:11:ASN:ND2 | 0.54 | 2.41 | 7 | 7 |
| 1:A:81:ALA:CB | 1:A:93:TYR:CG | 0.53 | 2.91 | 19 | 20 |
| 1:A:65:CYS:O | 1:A:67:HIS:ND1 | 0.53 | 2.41 | 7 | 8 |
| 1:A:70:GLN:O | 1:A:72:ARG:NH1 | 0.53 | 2.41 | 18 | 1 |
| 1:A:40:CYS:O | 1:A:42:GLU:N | 0.53 | 2.42 | 3 | 19 |
| 1:A:62:HIS:O | 1:A:64:ALA:N | 0.53 | 2.42 | 19 | 19 |
| 1:A:76:VAL:O | 1:A:78:LYS:N | 0.52 | 2.42 | 4 | 20 |
| 1:A:91:ASP:O | 1:A:95:ASN:ND2 | 0.52 | 2.43 | 19 | 4 |
| 1:A:41:GLU:OE2 | 1:A:61:TRP:CZ2 | 0.52 | 2.62 | 14 | 9 |
| 1:A:38:ASN:OD1 | 1:A:60:HIS:CE1 | 0.52 | 2.62 | 18 | 1 |
| 1:A:54:LEU:N | 1:A:61:TRP:O | 0.52 | 2.43 | 16 | 8 |
| 1:A:15:PHE:O | 1:A:17:LYS:N | 0.51 | 2.44 | 14 | 20 |
| 1:A:66:PHE:CE1 | 1:A:87:LEU:HD13 | 0.51 | 2.40 | 20 | 20 |
| 1:A:65:CYS:O | 1:A:67:HIS:CE1 | 0.51 | 2.64 | 9 | 9 |
| 1:A:45:LYS:CB | 1:A:45:LYS:NZ | 0.51 | 2.73 | 16 | 1 |
| 1:A:72:ARG:CG | 1:A:72:ARG:HH11 | 0.51 | 2.17 | 8 | 3 |
| 1:A:9:HIS:CD2 | 1:A:31:CYS:SG | 0.51 | 3.04 | 7 | 8 |
| 1:A:9:HIS:ND1 | 1:A:9:HIS:C | 0.51 | 2.64 | 3 | 20 |
| 1:A:91:ASP:N | 1:A:91:ASP:OD1 | 0.51 | 2.44 | 12 | 1 |
| 1:A:89:CYS:C | 1:A:91:ASP:N | 0.51 | 2.64 | 6 | 20 |
| 1:A:72:ARG:CG | 1:A:72:ARG:NH1 | 0.51 | 2.72 | 16 | 2 |
| 1:A:76:VAL:C | 1:A:78:LYS:N | 0.50 | 2.65 | 4 | 20 |
| 1:A:85:ASP:O | 1:A:86:GLN:NE2 | 0.50 | 2.44 | 6 | 1 |
| 1:A:84:GLU:H | 1:A:84:GLU:CD | 0.50 | 2.10 | 6 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:53:ASP:OD1 | 1:A:53:ASP:N | 0.49 | 2.43 | 13 | 8 |
| 1:A:14:LEU:N | 1:A:14:LEU:CD2 | 0.49 | 2.75 | 10 | 20 |
| 1:A:6:ASP:N | 1:A:6:ASP:OD1 | 0.49 | 2.45 | 10 | 1 |
| 1:A:22:ARG:NE | 1:A:36:PHE:CZ | 0.49 | 2.81 | 19 | 3 |
| 1:A:50:ASP:O | 1:A:51:CYS:SG | 0.49 | 2.70 | 5 | 5 |
| 1:A:62:HIS:O | 1:A:65:CYS:N | 0.48 | 2.46 | 19 | 18 |
| 1:A:38:ASN:CG | 1:A:60:HIS:CE1 | 0.48 | 2.87 | 10 | 18 |
| 1:A:10:CYS:O | 1:A:11:ASN:OD1 | 0.48 | 2.32 | 13 | 10 |
| 1:A:96:GLU:CD | 1:A:97:TYR:N | 0.48 | 2.67 | 16 | 2 |
| 1:A:72:ARG:NH1 | 1:A:72:ARG:CG | 0.48 | 2.74 | 19 | 1 |
| 1:A:57:LYS:O | 1:A:59:ARG:N | 0.48 | 2.47 | 1 | 3 |
| 1:A:33:GLU:O | 1:A:37:ALA:CB | 0.47 | 2.62 | 2 | 20 |
| 1:A:22:ARG:HH11 | 1:A:22:ARG:HG2 | 0.47 | 1.69 | 3 | 2 |
| 1:A:38:ASN:OD1 | 1:A:60:HIS:CD2 | 0.47 | 2.67 | 5 | 5 |
| 1:A:71:CYS:C | 1:A:73:ASN:N | 0.47 | 2.68 | 11 | 19 |
| 1:A:96:GLU:OE1 | 1:A:97:TYR:N | 0.47 | 2.47 | 10 | 1 |
| 1:A:22:ARG:N | 1:A:25:SER:O | 0.47 | 2.45 | 1 | 2 |
| 1:A:22:ARG:O | 1:A:25:SER:N | 0.47 | 2.46 | 7 | 3 |
| 1:A:45:LYS:CD | 1:A:45:LYS:N | 0.47 | 2.77 | 2 | 1 |
| 1:A:97:TYR:C | 1:A:97:TYR:CD1 | 0.47 | 2.87 | 3 | 1 |
| 1:A:19:TYR:N | 1:A:19:TYR:CD1 | 0.46 | 2.83 | 6 | 16 |
| 1:A:93:TYR:CE2 | 1:A:97:TYR:CG | 0.46 | 3.02 | 19 | 1 |
| 1:A:34:THR:CG2 | 1:A:35:LEU:N | 0.46 | 2.79 | 13 | 20 |
| 1:A:96:GLU:OE1 | 1:A:96:GLU:CA | 0.46 | 2.64 | 5 | 2 |
| 1:A:14:LEU:CD2 | 1:A:14:LEU:H | 0.45 | 2.25 | 8 | 20 |
| 1:A:62:HIS:C | 1:A:64:ALA:N | 0.45 | 2.70 | 19 | 6 |
| 1:A:11:ASN:O | 1:A:11:ASN:OD1 | 0.45 | 2.34 | 11 | 5 |
| 1:A:19:TYR:CD1 | 1:A:19:TYR:N | 0.45 | 2.85 | 11 | 4 |
| 1:A:17:LYS:CG | 1:A:18:LYS:N | 0.45 | 2.80 | 3 | 19 |
| 1:A:84:GLU:CD | 1:A:84:GLU:N | 0.45 | 2.70 | 6 | 3 |
| 1:A:11:ASN:CG | 1:A:11:ASN:O | 0.44 | 2.56 | 19 | 5 |
| 1:A:9:HIS:C | 1:A:9:HIS:HD1 | 0.44 | 2.16 | 11 | 2 |
| 1:A:18:LYS:CG | 1:A:19:TYR:N | 0.44 | 2.80 | 17 | 1 |
| 1:A:40:CYS:C | 1:A:42:GLU:N | 0.44 | 2.71 | 8 | 16 |
| 1:A:7:CYS:O | 1:A:9:HIS:N | 0.44 | 2.51 | 18 | 11 |
| 1:A:83:LYS:O | 1:A:84:GLU:C | 0.44 | 2.56 | 7 | 20 |
| 1:A:23:GLU:O | 1:A:24:GLU:CG | 0.44 | 2.66 | 1 | 2 |
| 1:A:62:HIS:O | 1:A:63:GLU:C | 0.43 | 2.56 | 2 | 19 |
| 1:A:15:PHE:O | 1:A:15:PHE:CG | 0.43 | 2.70 | 13 | 16 |
| 1:A:19:TYR:CE2 | 1:A:21:LEU:HD21 | 0.43 | 2.48 | 7 | 5 |
| 1:A:28:CYS:O | 1:A:29:VAL:C | 0.43 | 2.57 | 14 | 18 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:96:GLU:N | 1:A:96:GLU:CD | 0.43 | 2.70 | 5 | 1 |
| 1:A:50:ASP:C | 1:A:51:CYS:SG | 0.43 | 2.97 | 1 | 2 |
| 1:A:10:CYS:O | 1:A:11:ASN:CG | 0.43 | 2.57 | 7 | 7 |
| 1:A:15:PHE:CD1 | 1:A:15:PHE:N | 0.43 | 2.86 | 7 | 9 |
| 1:A:54:LEU:CB | 1:A:61:TRP:O | 0.43 | 2.67 | 17 | 16 |
| 1:A:10:CYS:O | 1:A:11:ASN:CB | 0.43 | 2.67 | 13 | 3 |
| 1:A:11:ASN:O | 1:A:11:ASN:CG | 0.43 | 2.56 | 4 | 1 |
| 1:A:58:ASP:OD1 | 1:A:58:ASP:O | 0.43 | 2.37 | 7 | 1 |
| 1:A:76:VAL:O | 1:A:77:ASP:CG | 0.42 | 2.58 | 10 | 5 |
| 1:A:14:LEU:HD22 | 1:A:14:LEU:H | 0.42 | 1.75 | 8 | 4 |
| 1:A:52:LYS:O | 1:A:63:GLU:OE1 | 0.42 | 2.37 | 11 | 1 |
| 1:A:97:TYR:O | 1:A:98:SER:O | 0.42 | 2.37 | 16 | 2 |
| 1:A:63:GLU:OE1 | 1:A:63:GLU:O | 0.42 | 2.36 | 1 | 1 |
| 1:A:42:GLU:O | 1:A:42:GLU:OE2 | 0.42 | 2.38 | 3 | 1 |
| 1:A:76:VAL:O | 1:A:77:ASP:OD2 | 0.42 | 2.38 | 10 | 1 |
| 1:A:40:CYS:O | 1:A:44:GLY:N | 0.42 | 2.52 | 20 | 3 |
| 1:A:8:HIS:O | 1:A:8:HIS:ND1 | 0.42 | 2.53 | 4 | 1 |
| 1:A:63:GLU:OE1 | 1:A:63:GLU:N | 0.42 | 2.53 | 11 | 1 |
| 1:A:96:GLU:OE2 | 1:A:97:TYR:N | 0.42 | 2.53 | 11 | 1 |
| 1:A:80:PHE:CD1 | 1:A:80:PHE:O | 0.41 | 2.73 | 11 | 1 |
| 1:A:89:CYS:O | 1:A:92:CYS:N | 0.41 | 2.53 | 11 | 1 |
| 1:A:22:ARG:HG2 | 1:A:27:TYR:CE2 | 0.41 | 2.50 | 3 | 3 |
| 1:A:49:CYS:C | 1:A:51:CYS:H | 0.41 | 2.19 | 8 | 4 |
| 1:A:76:VAL:C | 1:A:78:LYS:H | 0.41 | 2.17 | 4 | 5 |
| 1:A:18:LYS:N | 1:A:18:LYS:CD | 0.41 | 2.83 | 5 | 1 |
| 1:A:83:LYS:CG | 1:A:84:GLU:N | 0.41 | 2.84 | 10 | 9 |
| 1:A:11:ASN:OD1 | 1:A:11:ASN:C | 0.41 | 2.59 | 13 | 2 |
| 1:A:52:LYS:HZ2 | 1:A:52:LYS:HB3 | 0.41 | 1.74 | 9 | 1 |
| 1:A:30:VAL:O | 1:A:31:CYS:C | 0.41 | 2.59 | 3 | 3 |
| 1:A:89:CYS:O | 1:A:90:THR:C | 0.41 | 2.59 | 9 | 9 |
| 1:A:71:CYS:O | 1:A:72:ARG:C | 0.41 | 2.58 | 11 | 1 |
| 1:A:96:GLU:CD | 1:A:96:GLU:N | 0.40 | 2.74 | 3 | 1 |
| 1:A:22:ARG:HG2 | 1:A:27:TYR:CD2 | 0.40 | 2.51 | 4 | 2 |
| 1:A:89:CYS:C | 1:A:91:ASP:H | 0.40 | 2.19 | 8 | 5 |
| 1:A:58:ASP:O | 1:A:58:ASP:OD2 | 0.40 | 2.39 | 4 | 1 |
| 1:A:97:TYR:CD1 | 1:A:97:TYR:C | 0.40 | 2.95 | 11 | 1 |
| 1:A:84:GLU:N | 1:A:84:GLU:OE1 | 0.40 | 2.54 | 11 | 1 |
| 1:A:41:GLU:OE2 | 1:A:61:TRP:CH2 | 0.40 | 2.74 | 14 | 1 |
| 1:A:93:TYR:CE2 | 1:A:97:TYR:CD1 | 0.40 | 3.09 | 19 | 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 | 93/98 (95%) | 75±1 (81±1%) | 13±1 (14±1%) | 5±1 (5±1%) | 3 | 24 |
| All | All | 1860/1960 (95%) | 1504 (81%) | 263 (14%) | 93 (5%) | 3 | 24 |

All 8 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 | 16 | GLY | 20 |
| 1 | A | 90 | THR | 18 |
| 1 | A | 41 | GLU | 16 |
| 1 | A | 18 | LYS | 14 |
| 1 | A | 63 | GLU | 11 |
| 1 | A | 72 | ARG | 7 |
| 1 | A | 58 | ASP | 5 |
| 1 | A | 8 | HIS | 2 |

6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|--------------|-------------|----|
| 1 | A | 87/91 (96%) | 77±2 (89±2%) | 10±2 (11±2%) | 7 | 51 |
| All | All | 1740/1820 (96%) | 1541 (89%) | 199 (11%) | 7 | 51 |

All 25 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 9 | HIS | 20 |
| 1 | A | 36 | PHE | 20 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 54 | LEU | 20 |
| 1 | A | 61 | TRP | 20 |
| 1 | A | 90 | THR | 15 |
| 1 | A | 67 | HIS | 15 |
| 1 | A | 42 | GLU | 12 |
| 1 | A | 22 | ARG | 10 |
| 1 | A | 11 | ASN | 10 |
| 1 | A | 34 | THR | 8 |
| 1 | A | 25 | SER | 7 |
| 1 | A | 52 | LYS | 7 |
| 1 | A | 85 | ASP | 5 |
| 1 | A | 6 | ASP | 4 |
| 1 | A | 77 | ASP | 4 |
| 1 | A | 96 | GLU | 4 |
| 1 | A | 18 | LYS | 4 |
| 1 | A | 72 | ARG | 4 |
| 1 | A | 95 | ASN | 2 |
| 1 | A | 45 | LYS | 2 |
| 1 | A | 84 | GLU | 2 |
| 1 | A | 17 | LYS | 1 |
| 1 | A | 91 | ASP | 1 |
| 1 | A | 53 | ASP | 1 |
| 1 | A | 57 | LYS | 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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 79% for the well-defined parts and 79% 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

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 | 1010 |
| Number of shifts mapped to atoms | 1010 |
| 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

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 98 | -0.53 ± 0.15 | Should be checked |
| $^{13}\text{C}_\beta$ | 95 | 0.09 ± 0.27 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 93 | -0.71 ± 0.51 | None needed (imprecise) |

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 79%, i.e. 965 atoms were assigned a chemical shift out of a possible 1222. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 372/467 (80%) | 188/188 (100%) | 94/188 (50%) | 90/91 (99%) |
| Sidechain | 496/603 (82%) | 324/385 (84%) | 165/196 (84%) | 7/22 (32%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 97/152 (64%) | 66/76 (87%) | 30/70 (43%) | 1/6 (17%) |
| Overall | 965/1222 (79%) | 578/649 (89%) | 289/454 (64%) | 98/119 (82%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1010 atoms were assigned a chemical shift out of a possible 1283. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 386/487 (79%) | 195/196 (99%) | 98/196 (50%) | 93/95 (98%) |
| Sidechain | 527/644 (82%) | 345/411 (84%) | 175/208 (84%) | 7/25 (28%) |
| Aromatic | 97/152 (64%) | 66/76 (87%) | 30/70 (43%) | 1/6 (17%) |
| Overall | 1010/1283 (79%) | 606/683 (89%) | 303/474 (64%) | 101/126 (80%) |

7.1.4 Statistically unusual chemical shifts ⓘ

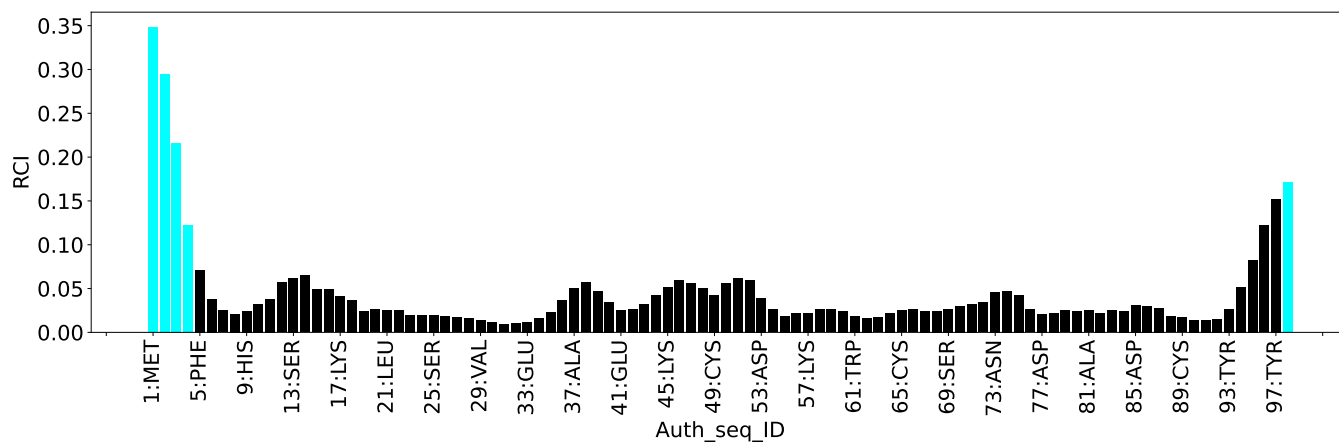
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 35 | LEU | HB2 | -0.44 | -0.07 – 3.30 | -6.1 |

7.1.5 Random Coil Index (RCI) plots ⓘ

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 | 1903 |
| Intra-residue ($ i-j =0$) | 577 |
| Sequential ($ i-j =1$) | 485 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 255 |
| Long range ($ i-j \geq 5$) | 586 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 190 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 20.7 |
| Number of long range restraints per residue ¹ | 5.8 |

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) | 40.7 | 0.2 |
| 0.2-0.5 (Medium) | 17.4 | 0.5 |
| >0.5 (Large) | 105.5 | 4.21 |

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) | 27.4 | 5.72 |
| 10.0-20.0 (Medium) | 2.0 | 15.57 |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

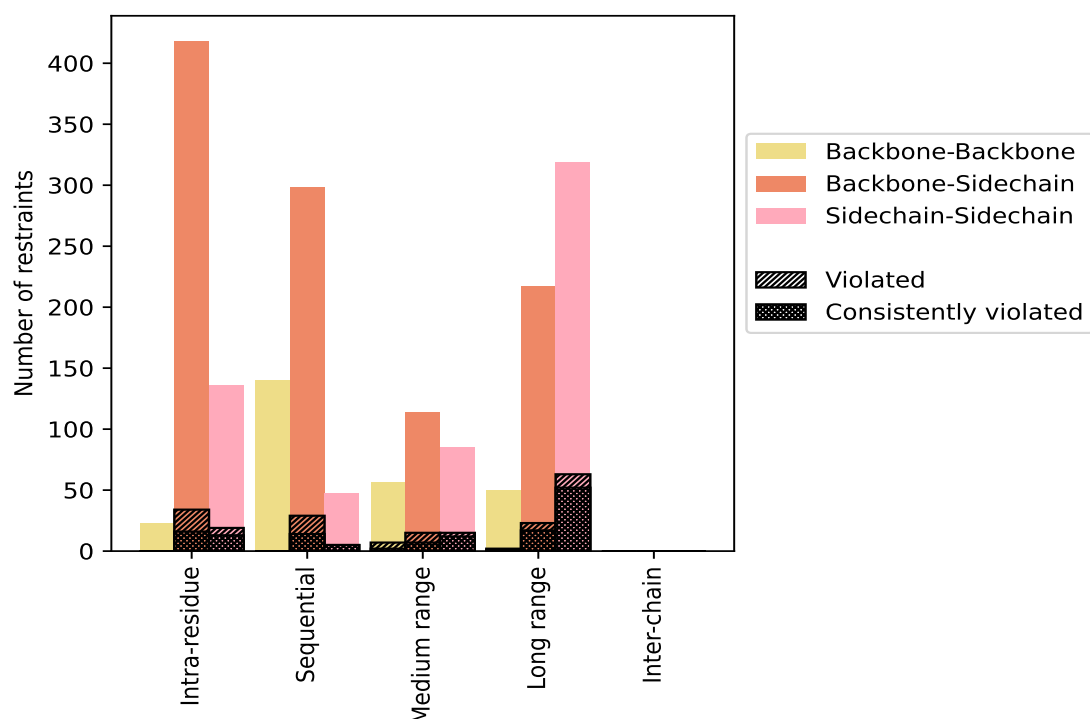
9.1 Summary of distance violations ⓘ

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) | 577 | 30.3 | 53 | 9.2 | 2.8 | 29 | 5.0 | 1.5 |
| Backbone-Backbone | 23 | 1.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 418 | 22.0 | 34 | 8.1 | 1.8 | 16 | 3.8 | 0.8 |
| Sidechain-Sidechain | 136 | 7.1 | 19 | 14.0 | 1.0 | 13 | 9.6 | 0.7 |
| Sequential (i-j =1) | 485 | 25.5 | 34 | 7.0 | 1.8 | 19 | 3.9 | 1.0 |
| Backbone-Backbone | 140 | 7.4 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 298 | 15.7 | 29 | 9.7 | 1.5 | 14 | 4.7 | 0.7 |
| Sidechain-Sidechain | 47 | 2.5 | 5 | 10.6 | 0.3 | 5 | 10.6 | 0.3 |
| Medium range (i-j >1 & i-j <5) | 255 | 13.4 | 37 | 14.5 | 1.9 | 21 | 8.2 | 1.1 |
| Backbone-Backbone | 56 | 2.9 | 7 | 12.5 | 0.4 | 2 | 3.6 | 0.1 |
| Backbone-Sidechain | 114 | 6.0 | 15 | 13.2 | 0.8 | 7 | 6.1 | 0.4 |
| Sidechain-Sidechain | 85 | 4.5 | 15 | 17.6 | 0.8 | 12 | 14.1 | 0.6 |
| Long range (i-j ≥5) | 586 | 30.8 | 88 | 15.0 | 4.6 | 70 | 11.9 | 3.7 |
| Backbone-Backbone | 50 | 2.6 | 2 | 4.0 | 0.1 | 1 | 2.0 | 0.1 |
| Backbone-Sidechain | 217 | 11.4 | 23 | 10.6 | 1.2 | 17 | 7.8 | 0.9 |
| Sidechain-Sidechain | 319 | 16.8 | 63 | 19.7 | 3.3 | 52 | 16.3 | 2.7 |
| 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 | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 1903 | 100.0 | 212 | 11.1 | 11.1 | 139 | 7.3 | 7.3 |
| Backbone-Backbone | 269 | 14.1 | 9 | 3.3 | 0.5 | 3 | 1.1 | 0.2 |
| Backbone-Sidechain | 1047 | 55.0 | 101 | 9.6 | 5.3 | 54 | 5.2 | 2.8 |
| Sidechain-Sidechain | 587 | 30.8 | 102 | 17.4 | 5.4 | 82 | 14.0 | 4.3 |

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 | 38 | 27 | 27 | 77 | 0 | 169 | 1.46 | 4.19 | 1.31 | 1.13 |
| 2 | 41 | 25 | 28 | 76 | 0 | 170 | 1.45 | 4.18 | 1.3 | 1.13 |
| 3 | 37 | 26 | 26 | 76 | 0 | 165 | 1.46 | 4.21 | 1.31 | 1.08 |
| 4 | 42 | 25 | 29 | 76 | 0 | 172 | 1.45 | 4.18 | 1.3 | 1.16 |
| 5 | 41 | 26 | 27 | 77 | 0 | 171 | 1.46 | 4.2 | 1.29 | 1.16 |
| 6 | 40 | 27 | 26 | 76 | 0 | 169 | 1.46 | 4.2 | 1.29 | 1.18 |
| 7 | 39 | 25 | 28 | 79 | 0 | 171 | 1.44 | 4.2 | 1.31 | 1.07 |
| 8 | 41 | 24 | 23 | 78 | 0 | 166 | 1.52 | 4.18 | 1.29 | 1.35 |
| 9 | 36 | 23 | 26 | 79 | 0 | 164 | 1.53 | 4.19 | 1.29 | 1.33 |
| 10 | 40 | 26 | 27 | 80 | 0 | 173 | 1.46 | 4.19 | 1.3 | 1.22 |

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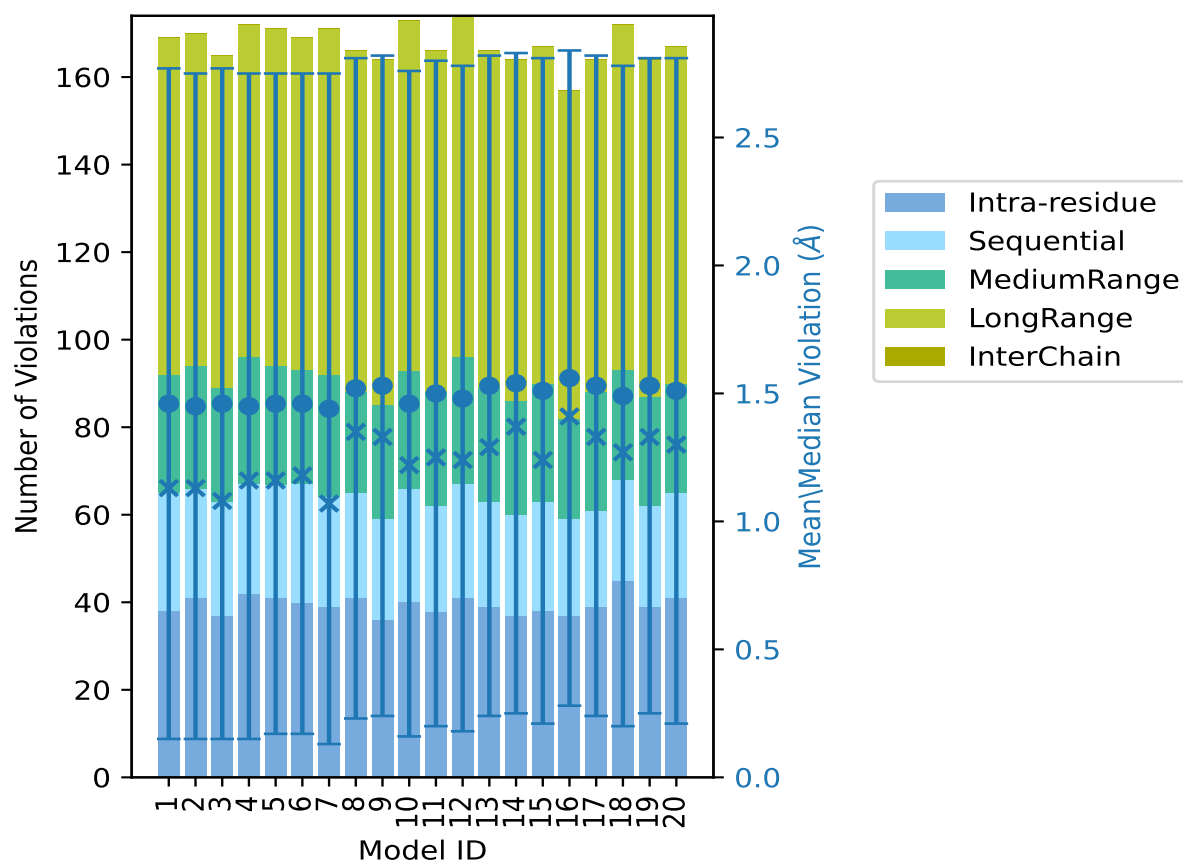
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 38 | 24 | 26 | 78 | 0 | 166 | 1.5 | 4.19 | 1.3 | 1.25 |
| 12 | 41 | 26 | 29 | 78 | 0 | 174 | 1.48 | 4.19 | 1.3 | 1.24 |
| 13 | 39 | 24 | 26 | 77 | 0 | 166 | 1.53 | 4.18 | 1.29 | 1.29 |
| 14 | 37 | 23 | 26 | 78 | 0 | 164 | 1.54 | 4.17 | 1.29 | 1.37 |
| 15 | 38 | 25 | 27 | 77 | 0 | 167 | 1.51 | 4.19 | 1.3 | 1.24 |
| 16 | 37 | 22 | 23 | 75 | 0 | 157 | 1.56 | 4.17 | 1.28 | 1.41 |
| 17 | 39 | 22 | 27 | 76 | 0 | 164 | 1.53 | 4.19 | 1.29 | 1.33 |
| 18 | 45 | 23 | 25 | 79 | 0 | 172 | 1.49 | 4.18 | 1.29 | 1.27 |
| 19 | 39 | 23 | 25 | 77 | 0 | 164 | 1.53 | 4.18 | 1.28 | 1.33 |
| 20 | 41 | 24 | 25 | 77 | 0 | 167 | 1.51 | 4.18 | 1.3 | 1.3 |

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

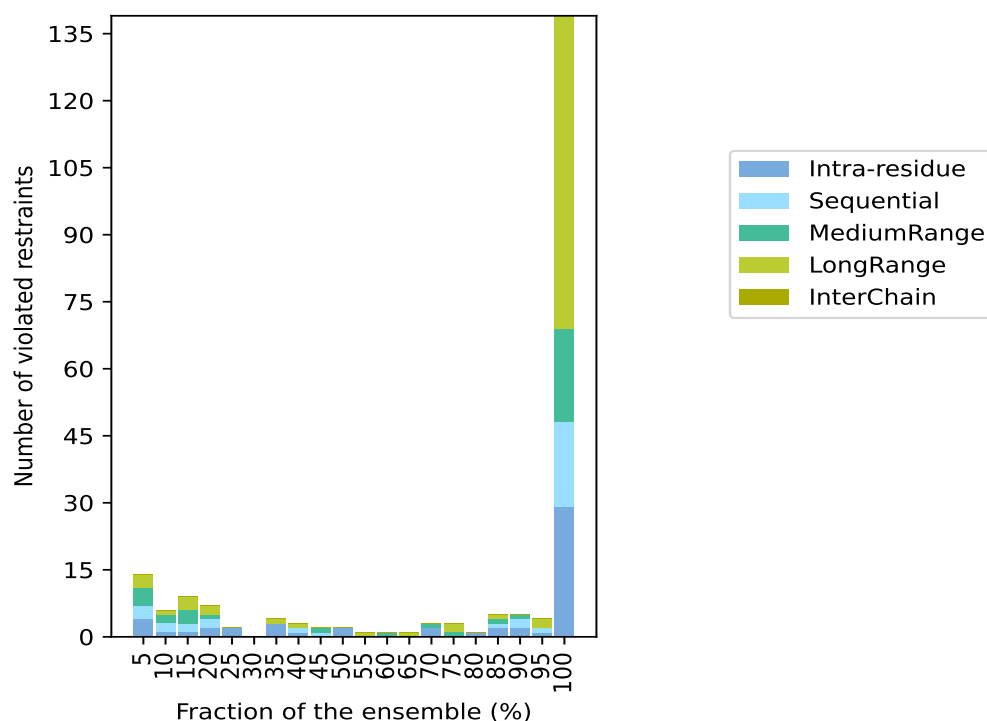
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1691(IR:524, SQ:451, MR:218, LR:498, IC:0) restraints are 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 | % |
| 4 | 3 | 4 | 3 | 0 | 14 | 1 | 5.0 |
| 1 | 2 | 2 | 1 | 0 | 6 | 2 | 10.0 |
| 1 | 2 | 3 | 3 | 0 | 9 | 3 | 15.0 |
| 2 | 2 | 1 | 2 | 0 | 7 | 4 | 20.0 |
| 2 | 0 | 0 | 0 | 0 | 2 | 5 | 25.0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 6 | 30.0 |
| 3 | 0 | 0 | 1 | 0 | 4 | 7 | 35.0 |
| 1 | 1 | 0 | 1 | 0 | 3 | 8 | 40.0 |
| 0 | 1 | 1 | 0 | 0 | 2 | 9 | 45.0 |
| 2 | 0 | 0 | 0 | 0 | 2 | 10 | 50.0 |
| 0 | 0 | 0 | 1 | 0 | 1 | 11 | 55.0 |
| 0 | 0 | 1 | 0 | 0 | 1 | 12 | 60.0 |
| 0 | 0 | 0 | 1 | 0 | 1 | 13 | 65.0 |
| 2 | 0 | 1 | 0 | 0 | 3 | 14 | 70.0 |
| 0 | 0 | 1 | 2 | 0 | 3 | 15 | 75.0 |
| 1 | 0 | 0 | 0 | 0 | 1 | 16 | 80.0 |
| 2 | 1 | 1 | 1 | 0 | 5 | 17 | 85.0 |
| 2 | 2 | 1 | 0 | 0 | 5 | 18 | 90.0 |
| 1 | 1 | 0 | 2 | 0 | 4 | 19 | 95.0 |
| 29 | 19 | 21 | 70 | 0 | 139 | 20 | 100.0 |

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

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

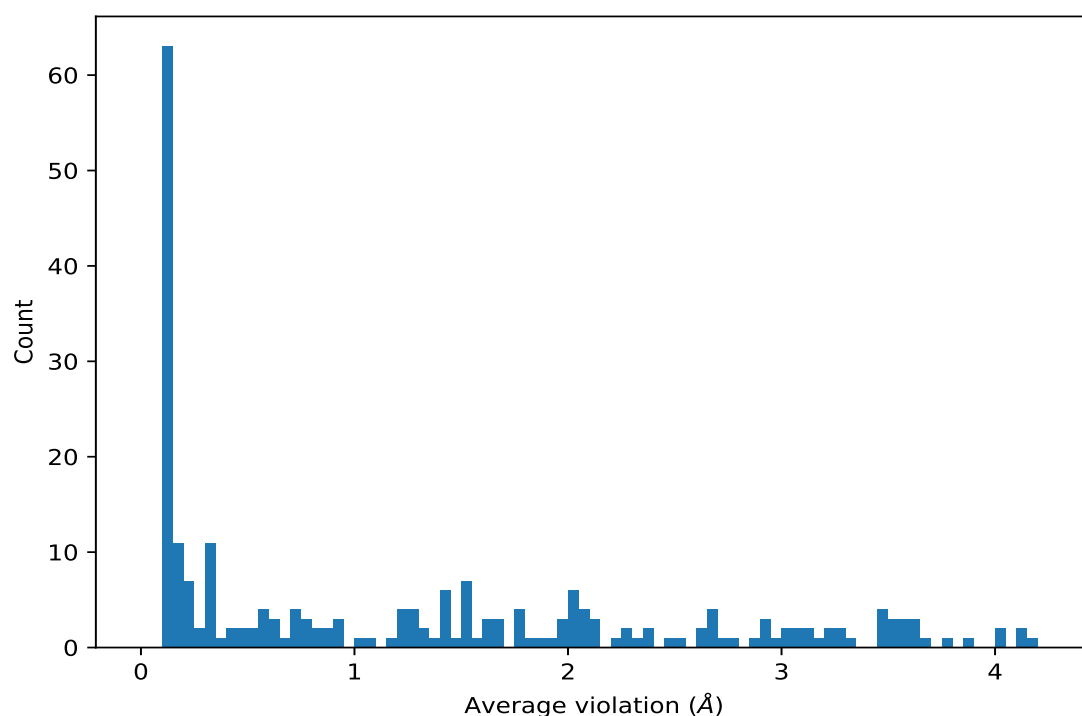
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 20 | 4.19 | 0.01 | 4.19 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 20 | 4.11 | 0.01 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 20 | 4.11 | 0.01 | 4.11 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 20 | 4.04 | 0.02 | 4.04 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 20 | 4.01 | 0.08 | 3.99 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 20 | 3.89 | 0.07 | 3.87 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 20 | 3.78 | 0.01 | 3.78 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 20 | 3.69 | 0.01 | 3.69 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 20 | 3.63 | 0.09 | 3.63 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 20 | 3.62 | 0.08 | 3.62 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 20 | 3.61 | 0.07 | 3.61 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 20 | 3.58 | 0.03 | 3.59 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 20 | 3.57 | 0.25 | 3.47 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 20 | 3.57 | 0.01 | 3.57 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 20 | 3.55 | 0.01 | 3.55 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 20 | 3.53 | 0.01 | 3.53 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 20 | 3.53 | 0.03 | 3.53 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 20 | 3.49 | 0.1 | 3.51 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 20 | 3.49 | 0.07 | 3.49 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 20 | 3.46 | 0.11 | 3.51 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 20 | 3.45 | 0.12 | 3.49 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 20 | 3.34 | 0.04 | 3.32 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 20 | 3.29 | 0.05 | 3.3 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 20 | 3.27 | 0.22 | 3.18 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 20 | 3.24 | 0.03 | 3.24 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 20 | 3.2 | 0.05 | 3.2 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 20 | 3.17 | 0.26 | 3.2 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 20 | 3.14 | 0.03 | 3.14 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 20 | 3.1 | 0.04 | 3.1 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 20 | 3.07 | 0.02 | 3.08 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 20 | 3.07 | 0.04 | 3.08 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 20 | 3.04 | 0.02 | 3.04 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 20 | 3.03 | 0.12 | 3.09 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 20 | 2.95 | 0.02 | 2.94 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 20 | 2.92 | 0.26 | 3.06 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 20 | 2.91 | 0.03 | 2.9 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 20 | 2.91 | 0.03 | 2.9 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 20 | 2.86 | 0.02 | 2.86 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 20 | 2.77 | 0.04 | 2.78 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 20 | 2.69 | 0.04 | 2.7 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 20 | 2.66 | 0.04 | 2.65 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 20 | 2.66 | 0.3 | 2.84 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 20 | 2.62 | 0.24 | 2.52 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 20 | 2.61 | 0.04 | 2.62 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 20 | 2.53 | 0.02 | 2.53 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 20 | 2.47 | 0.09 | 2.46 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 20 | 2.37 | 0.08 | 2.38 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 20 | 2.36 | 0.04 | 2.37 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 20 | 2.31 | 0.05 | 2.32 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 20 | 2.29 | 0.11 | 2.28 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 20 | 2.27 | 0.04 | 2.26 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 20 | 2.24 | 0.78 | 2.72 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 20 | 2.11 | 0.1 | 2.09 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 20 | 2.11 | 0.1 | 2.09 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 20 | 2.11 | 0.1 | 2.09 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 20 | 2.08 | 0.21 | 2.0 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 20 | 2.07 | 0.03 | 2.07 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 20 | 2.07 | 0.03 | 2.07 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 20 | 2.07 | 0.03 | 2.07 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 20 | 2.04 | 0.03 | 2.05 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 20 | 2.04 | 0.03 | 2.05 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 20 | 2.04 | 0.03 | 2.05 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 20 | 2.03 | 0.02 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 20 | 2.03 | 0.02 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 20 | 2.03 | 0.02 | 2.03 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 20 | 1.99 | 0.05 | 1.98 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 20 | 1.99 | 0.05 | 1.98 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 20 | 1.98 | 0.03 | 1.98 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 20 | 1.93 | 0.05 | 1.92 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 20 | 1.86 | 0.12 | 1.8 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 20 | 1.83 | 0.01 | 1.84 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 20 | 1.78 | 0.07 | 1.76 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 20 | 1.78 | 0.09 | 1.78 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 20 | 1.78 | 0.09 | 1.78 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 20 | 1.78 | 0.09 | 1.78 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 20 | 1.68 | 0.19 | 1.7 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 20 | 1.67 | 0.04 | 1.65 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 20 | 1.67 | 0.23 | 1.74 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 20 | 1.61 | 0.05 | 1.62 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 20 | 1.61 | 0.05 | 1.62 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 20 | 1.61 | 0.05 | 1.62 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 20 | 1.58 | 0.03 | 1.59 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 20 | 1.54 | 0.09 | 1.52 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 20 | 1.51 | 0.25 | 1.61 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 20 | 1.5 | 0.07 | 1.54 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 20 | 1.5 | 0.02 | 1.5 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 20 | 1.5 | 0.09 | 1.5 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 20 | 1.5 | 0.09 | 1.5 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 20 | 1.5 | 0.09 | 1.5 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 20 | 1.48 | 0.27 | 1.28 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 20 | 1.44 | 0.03 | 1.44 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 20 | 1.44 | 0.03 | 1.44 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 20 | 1.44 | 0.03 | 1.44 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 20 | 1.43 | 0.11 | 1.42 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 20 | 1.41 | 0.02 | 1.41 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 20 | 1.36 | 0.21 | 1.45 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 20 | 1.34 | 0.06 | 1.31 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 20 | 1.32 | 0.06 | 1.32 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 20 | 1.26 | 0.03 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 20 | 1.26 | 0.03 | 1.27 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 20 | 1.26 | 0.03 | 1.27 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 20 | 1.25 | 0.17 | 1.31 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 20 | 1.24 | 0.06 | 1.27 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 20 | 1.21 | 0.04 | 1.21 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 20 | 1.21 | 0.04 | 1.21 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 20 | 1.21 | 0.04 | 1.21 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 20 | 1.18 | 0.15 | 1.25 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 20 | 1.07 | 0.0 | 1.07 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 20 | 1.03 | 0.06 | 1.02 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 20 | 0.95 | 0.11 | 0.93 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 20 | 0.95 | 0.0 | 0.95 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 20 | 0.92 | 0.26 | 0.83 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 20 | 0.88 | 0.09 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 20 | 0.86 | 0.01 | 0.86 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 20 | 0.84 | 0.16 | 0.84 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 20 | 0.79 | 0.0 | 0.79 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 20 | 0.79 | 0.04 | 0.8 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 20 | 0.76 | 0.01 | 0.76 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 20 | 0.74 | 0.02 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 20 | 0.73 | 0.04 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 20 | 0.73 | 0.04 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 20 | 0.73 | 0.04 | 0.74 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 20 | 0.65 | 0.01 | 0.65 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 20 | 0.63 | 0.04 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 20 | 0.63 | 0.04 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 20 | 0.63 | 0.04 | 0.63 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 20 | 0.55 | 0.0 | 0.55 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 20 | 0.51 | 0.0 | 0.51 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 20 | 0.5 | 0.01 | 0.5 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 20 | 0.45 | 0.01 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 20 | 0.45 | 0.0 | 0.45 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 20 | 0.44 | 0.0 | 0.44 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 20 | 0.38 | 0.01 | 0.39 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 20 | 0.34 | 0.04 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 20 | 0.34 | 0.04 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 20 | 0.34 | 0.04 | 0.34 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 20 | 0.34 | 0.02 | 0.34 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 20 | 0.34 | 0.02 | 0.34 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 20 | 0.34 | 0.03 | 0.36 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 20 | 0.34 | 0.03 | 0.36 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 20 | 0.34 | 0.0 | 0.34 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 20 | 0.32 | 0.11 | 0.31 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 20 | 0.32 | 0.03 | 0.32 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 20 | 0.25 | 0.01 | 0.24 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 20 | 0.2 | 0.01 | 0.2 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 20 | 0.2 | 0.02 | 0.2 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 20 | 0.19 | 0.02 | 0.19 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 20 | 0.19 | 0.01 | 0.19 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 20 | 0.18 | 0.0 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 20 | 0.18 | 0.01 | 0.18 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 20 | 0.17 | 0.02 | 0.17 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 20 | 0.17 | 0.02 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 20 | 0.16 | 0.01 | 0.16 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 20 | 0.16 | 0.02 | 0.16 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 20 | 0.16 | 0.01 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 20 | 0.15 | 0.02 | 0.16 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 20 | 0.14 | 0.01 | 0.15 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 20 | 0.14 | 0.02 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 20 | 0.14 | 0.01 | 0.14 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 20 | 0.13 | 0.01 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 20 | 0.13 | 0.01 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 20 | 0.13 | 0.01 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 20 | 0.13 | 0.0 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 20 | 0.13 | 0.0 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 20 | 0.13 | 0.0 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 20 | 0.13 | 0.01 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 20 | 0.13 | 0.01 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 20 | 0.12 | 0.0 | 0.12 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 20 | 0.12 | 0.01 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 20 | 0.12 | 0.01 | 0.12 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 20 | 0.12 | 0.01 | 0.12 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 19 | 0.14 | 0.02 | 0.14 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 19 | 0.12 | 0.01 | 0.12 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 19 | 0.11 | 0.01 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 19 | 0.11 | 0.01 | 0.11 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 18 | 0.55 | 0.32 | 0.42 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 18 | 0.55 | 0.32 | 0.42 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 18 | 0.14 | 0.01 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 18 | 0.13 | 0.02 | 0.14 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 18 | 0.12 | 0.01 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 18 | 0.11 | 0.01 | 0.11 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 17 | 2.73 | 0.14 | 2.75 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 17 | 2.69 | 0.03 | 2.68 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 17 | 1.42 | 0.7 | 1.75 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 17 | 0.43 | 0.01 | 0.43 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 17 | 0.31 | 0.02 | 0.31 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 16 | 0.19 | 0.01 | 0.19 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 15 | 0.12 | 0.01 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 15 | 0.11 | 0.01 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 15 | 0.11 | 0.01 | 0.11 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 14 | 0.16 | 0.04 | 0.15 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 14 | 0.13 | 0.04 | 0.11 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 14 | 0.11 | 0.01 | 0.11 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 13 | 0.85 | 0.08 | 0.84 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 12 | 0.56 | 0.36 | 0.4 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 11 | 0.11 | 0.01 | 0.11 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 10 | 0.21 | 0.0 | 0.21 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 10 | 0.15 | 0.02 | 0.14 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 9 | 0.15 | 0.03 | 0.15 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 9 | 0.11 | 0.01 | 0.11 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 8 | 0.2 | 0.01 | 0.21 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 8 | 0.12 | 0.01 | 0.12 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 8 | 0.11 | 0.01 | 0.11 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 7 | 0.13 | 0.01 | 0.13 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 7 | 0.11 | 0.01 | 0.12 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 7 | 0.1 | 0.0 | 0.1 |
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 7 | 0.1 | 0.0 | 0.1 |
| (1,1203) | 1:59:A:ARG:HG2 | 1:59:A:ARG:HE | 5 | 0.25 | 0.02 | 0.26 |
| (1,518) | 1:22:A:ARG:HA | 1:22:A:ARG:HG3 | 5 | 0.23 | 0.06 | 0.26 |
| (1,738) | 1:33:A:GLU:HG2 | 1:34:A:THR:H | 4 | 0.22 | 0.01 | 0.22 |
| (1,1897) | 1:97:A:TYR:HB2 | 1:98:A:SER:H | 4 | 0.15 | 0.02 | 0.15 |
| (1,263) | 1:11:A:ASN:HB2 | 1:11:A:ASN:HD22 | 4 | 0.14 | 0.01 | 0.14 |
| (1,552) | 1:22:A:ARG:HD2 | 1:32:A:PHE:HD2 | 4 | 0.13 | 0.01 | 0.13 |
| (1,719) | 1:32:A:PHE:HA | 1:35:A:LEU:HG | 4 | 0.11 | 0.01 | 0.11 |
| (1,1137) | 1:56:A:TYR:HA | 1:56:A:TYR:HD1 | 4 | 0.11 | 0.01 | 0.11 |
| (1,1630) | 1:80:A:PHE:HB3 | 1:90:A:THR:H | 4 | 0.11 | 0.0 | 0.11 |
| (1,1044) | 1:52:A:LYS:HA | 1:52:A:LYS:HG3 | 3 | 0.24 | 0.0 | 0.24 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD21 | 3 | 0.12 | 0.02 | 0.12 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD22 | 3 | 0.12 | 0.02 | 0.12 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD23 | 3 | 0.12 | 0.02 | 0.12 |
| (1,402) | 1:18:A:LYS:HG3 | 1:19:A:TYR:H | 3 | 0.12 | 0.0 | 0.12 |
| (1,415) | 1:19:A:TYR:HA | 1:20:A:ILE:HG12 | 3 | 0.11 | 0.0 | 0.11 |
| (1,724) | 1:32:A:PHE:HA | 1:36:A:PHE:H | 3 | 0.11 | 0.01 | 0.11 |
| (1,677) | 1:30:A:VAL:HA | 1:33:A:GLU:H | 3 | 0.11 | 0.0 | 0.11 |
| (1,1460) | 1:70:A:GLN:HG3 | 1:88:A:LEU:HG | 3 | 0.1 | 0.0 | 0.1 |
| (1,1273) | 1:63:A:GLU:HA | 1:65:A:CYS:H | 3 | 0.1 | 0.0 | 0.1 |

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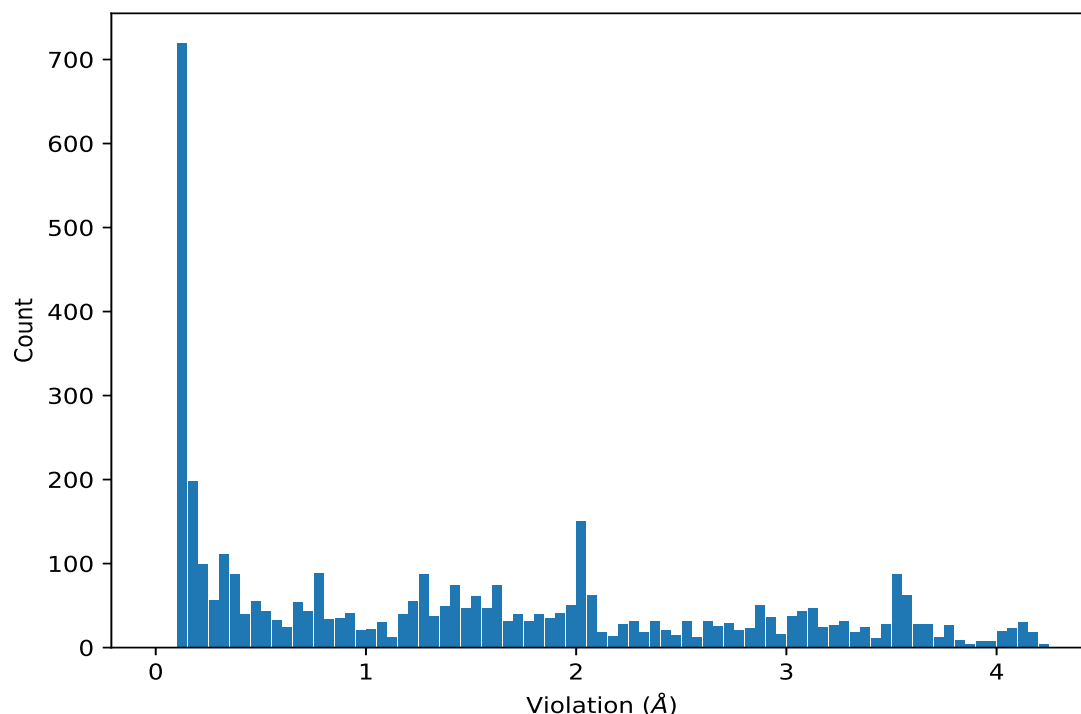
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|----------------|----------------|---------------------|----------|---------------------|------------|
| (1,1407) | 1:68:A:CYS:HB2 | 1:89:A:CYS:HA | 3 | 0.1 | 0.0 | 0.1 |
| (1,8) | 1:2:A:THR:HG21 | 1:3:A:GLU:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,8) | 1:2:A:THR:HG22 | 1:3:A:GLU:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,8) | 1:2:A:THR:HG23 | 1:3:A:GLU:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,9) | 1:2:A:THR:HB | 1:3:A:GLU:H | 2 | 0.12 | 0.0 | 0.12 |
| (1,51) | 1:4:A:ARG:HB3 | 1:6:A:ASP:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,655) | 1:29:A:VAL:HA | 1:32:A:PHE:HB2 | 2 | 0.11 | 0.0 | 0.11 |
| (1,826) | 1:38:A:ASN:HB3 | 1:38:A:ASN:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,1153) | 1:56:A:TYR:HB2 | 1:61:A:TRP:HZ3 | 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) |
|---------|----------------|----------------|----------|---------------|
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 3 | 4.21 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 5 | 4.2 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 6 | 4.2 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 7 | 4.2 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 1 | 4.19 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 9 | 4.19 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 10 | 4.19 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 11 | 4.19 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 12 | 4.19 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 15 | 4.19 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 17 | 4.19 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 2 | 4.18 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 4 | 4.18 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 8 | 4.18 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 13 | 4.18 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 18 | 4.18 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 19 | 4.18 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 20 | 4.18 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 14 | 4.17 |
| (1,363) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB3 | 16 | 4.17 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 1 | 4.16 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 7 | 4.16 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 3 | 4.14 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 2 | 4.13 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 4 | 4.13 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 5 | 4.13 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 6 | 4.13 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 10 | 4.13 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 3 | 4.12 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 5 | 4.12 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 7 | 4.12 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 15 | 4.12 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 1 | 4.12 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 9 | 4.12 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 12 | 4.12 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 17 | 4.12 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 1 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 2 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 6 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 9 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 10 | 4.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 11 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 12 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 13 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 14 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 17 | 4.11 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 7 | 4.11 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 11 | 4.11 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 13 | 4.11 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 14 | 4.11 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 15 | 4.11 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 16 | 4.11 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 4 | 4.1 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 8 | 4.1 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 18 | 4.1 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 19 | 4.1 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 20 | 4.1 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 3 | 4.1 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 8 | 4.1 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 18 | 4.1 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 19 | 4.1 |
| (1,200) | 1:8:A:HIS:H | 1:27:A:TYR:HD2 | 20 | 4.1 |
| (1,365) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB3 | 16 | 4.09 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 2 | 4.09 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 5 | 4.09 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 6 | 4.09 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 4 | 4.08 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 1 | 4.07 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 13 | 4.07 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 4 | 4.06 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 14 | 4.06 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 12 | 4.05 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 15 | 4.05 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 16 | 4.05 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 20 | 4.05 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 2 | 4.04 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 3 | 4.04 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 7 | 4.04 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 10 | 4.04 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 3 | 4.03 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 8 | 4.03 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 11 | 4.03 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 17 | 4.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 18 | 4.03 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 19 | 4.03 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 15 | 4.03 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 1 | 4.02 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 7 | 4.02 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 9 | 4.02 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 7 | 4.02 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 12 | 4.01 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 1 | 4.01 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 6 | 4.0 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 13 | 4.0 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 3 | 4.0 |
| (1,362) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HA | 5 | 3.99 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 10 | 3.98 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 9 | 3.96 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 17 | 3.96 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 16 | 3.95 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 20 | 3.95 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 2 | 3.95 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 5 | 3.95 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 6 | 3.94 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 11 | 3.93 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 18 | 3.93 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 19 | 3.93 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 4 | 3.93 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 8 | 3.92 |
| (1,199) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HE2 | 14 | 3.92 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 15 | 3.91 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 12 | 3.9 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 13 | 3.88 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 10 | 3.86 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 17 | 3.86 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 9 | 3.84 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 16 | 3.84 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 20 | 3.84 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 11 | 3.83 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 18 | 3.83 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 19 | 3.83 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 14 | 3.82 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 6 | 3.81 |
| (1,198) | 1:8:A:HIS:HB2 | 1:27:A:TYR:HD2 | 8 | 3.81 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 2 | 3.8 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 5 | 3.8 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 5 | 3.8 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 1 | 3.8 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 3 | 3.79 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 6 | 3.79 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 8 | 3.79 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 11 | 3.79 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 15 | 3.79 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 18 | 3.79 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 19 | 3.79 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 7 | 3.79 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 1 | 3.78 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 4 | 3.78 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 7 | 3.78 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 9 | 3.78 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 10 | 3.78 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 12 | 3.78 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 17 | 3.78 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 20 | 3.78 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 4 | 3.77 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 2 | 3.77 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 13 | 3.77 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 14 | 3.77 |
| (1,366) | 1:15:A:PHE:HE2 | 1:28:A:CYS:HB2 | 16 | 3.77 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 1 | 3.77 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 7 | 3.75 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 3 | 3.73 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 4 | 3.72 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 14 | 3.72 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 6 | 3.71 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 3 | 3.71 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 3 | 3.7 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 5 | 3.7 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 8 | 3.7 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 11 | 3.7 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 18 | 3.7 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 19 | 3.7 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 5 | 3.7 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 12 | 3.69 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 1 | 3.69 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 4 | 3.69 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 7 | 3.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 9 | 3.69 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 12 | 3.69 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 15 | 3.69 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 17 | 3.69 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 20 | 3.69 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 5 | 3.69 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 2 | 3.69 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 4 | 3.69 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 6 | 3.69 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 11 | 3.68 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 18 | 3.68 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 7 | 3.68 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 2 | 3.68 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 10 | 3.68 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 13 | 3.68 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 16 | 3.68 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 2 | 3.68 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 4 | 3.68 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 6 | 3.68 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 1 | 3.67 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 3 | 3.67 |
| (1,364) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HB2 | 14 | 3.67 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 10 | 3.67 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 1 | 3.66 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 16 | 3.65 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 13 | 3.65 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 5 | 3.64 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 12 | 3.64 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 11 | 3.63 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 10 | 3.63 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 9 | 3.62 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 8 | 3.62 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 9 | 3.62 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 12 | 3.62 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 13 | 3.62 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 8 | 3.62 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 15 | 3.62 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 3 | 3.61 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 13 | 3.61 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 15 | 3.61 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 3 | 3.61 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 13 | 3.61 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 14 | 3.61 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 20 | 3.61 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 15 | 3.61 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 6 | 3.6 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 14 | 3.6 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 12 | 3.6 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 15 | 3.6 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 18 | 3.6 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 8 | 3.6 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 9 | 3.6 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 4 | 3.59 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 2 | 3.59 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 7 | 3.59 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 16 | 3.59 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 13 | 3.59 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 14 | 3.59 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 7 | 3.58 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 10 | 3.58 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 15 | 3.58 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 15 | 3.58 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 17 | 3.58 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 14 | 3.58 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 20 | 3.58 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 8 | 3.57 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 19 | 3.57 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 11 | 3.57 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 13 | 3.57 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 1 | 3.57 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 3 | 3.57 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 10 | 3.57 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 17 | 3.57 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 4 | 3.57 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 1 | 3.57 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 4 | 3.57 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 13 | 3.57 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 2 | 3.57 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 9 | 3.57 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 10 | 3.57 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 11 | 3.57 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 12 | 3.57 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 16 | 3.57 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 18 | 3.57 |

Continued on next page...

Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 20 | 3.57 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 10 | 3.57 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 14 | 3.57 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 8 | 3.57 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 9 | 3.57 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 12 | 3.56 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 18 | 3.56 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 10 | 3.56 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 14 | 3.56 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 4 | 3.56 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 2 | 3.56 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 12 | 3.56 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 17 | 3.56 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 18 | 3.56 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 15 | 3.56 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 7 | 3.56 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 12 | 3.56 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 14 | 3.56 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 15 | 3.56 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 16 | 3.56 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 20 | 3.56 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 1 | 3.56 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 4 | 3.56 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 7 | 3.56 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 8 | 3.56 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 19 | 3.56 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 11 | 3.56 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 5 | 3.56 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 20 | 3.56 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 11 | 3.56 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 1 | 3.55 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 2 | 3.55 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 6 | 3.55 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 6 | 3.55 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 19 | 3.55 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 20 | 3.55 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 3 | 3.55 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 2 | 3.55 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 3 | 3.55 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 8 | 3.55 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 10 | 3.55 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 11 | 3.55 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 17 | 3.55 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 18 | 3.55 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 19 | 3.55 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 9 | 3.55 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 16 | 3.55 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 17 | 3.55 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 20 | 3.55 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 2 | 3.55 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 4 | 3.55 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 6 | 3.55 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 11 | 3.55 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 14 | 3.55 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 17 | 3.55 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 17 | 3.55 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 2 | 3.54 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 20 | 3.54 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 16 | 3.54 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 19 | 3.54 |
| (1,1251) | 1:61:A:TRP:HB2 | 1:66:A:PHE:HD1 | 5 | 3.54 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 1 | 3.54 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 7 | 3.54 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 18 | 3.54 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 9 | 3.54 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 13 | 3.54 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 9 | 3.54 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 3 | 3.54 |
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 5 | 3.54 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 19 | 3.54 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 1 | 3.54 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 10 | 3.54 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 17 | 3.54 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 16 | 3.54 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 16 | 3.54 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 7 | 3.53 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 8 | 3.53 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 11 | 3.53 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 7 | 3.53 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 10 | 3.53 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 20 | 3.53 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 12 | 3.53 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 11 | 3.53 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 6 | 3.53 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,309) | 1:14:A:LEU:HA | 1:15:A:PHE:HD2 | 6 | 3.53 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 9 | 3.53 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 12 | 3.53 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 13 | 3.53 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 15 | 3.53 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 5 | 3.52 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 9 | 3.52 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 15 | 3.52 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 20 | 3.52 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 12 | 3.52 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 12 | 3.52 |
| (1,361) | 1:15:A:PHE:HD2 | 1:28:A:CYS:HA | 5 | 3.52 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 18 | 3.52 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 7 | 3.52 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 11 | 3.52 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 14 | 3.52 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 16 | 3.52 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 18 | 3.52 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 20 | 3.52 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 17 | 3.51 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 18 | 3.51 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 11 | 3.51 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 19 | 3.51 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 3 | 3.51 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 8 | 3.51 |
| (1,201) | 1:8:A:HIS:H | 1:27:A:TYR:HE2 | 19 | 3.51 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 19 | 3.51 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 9 | 3.5 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 5 | 3.5 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 13 | 3.5 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 17 | 3.5 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 13 | 3.5 |
| (1,197) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HE2 | 18 | 3.5 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 19 | 3.5 |
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 16 | 3.49 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 6 | 3.49 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 13 | 3.49 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 12 | 3.49 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 14 | 3.49 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 15 | 3.49 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 17 | 3.49 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 12 | 3.49 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1707) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HE2 | 17 | 3.48 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 3 | 3.48 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 15 | 3.48 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 1 | 3.48 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 11 | 3.48 |
| (1,196) | 1:8:A:HIS:HB3 | 1:27:A:TYR:HD2 | 18 | 3.48 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 4 | 3.47 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 10 | 3.47 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 13 | 3.47 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 6 | 3.47 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 20 | 3.47 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 7 | 3.46 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 10 | 3.46 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 10 | 3.46 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 16 | 3.46 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 5 | 3.46 |
| (1,1317) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB3 | 1 | 3.45 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 2 | 3.45 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 15 | 3.45 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 15 | 3.45 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 8 | 3.44 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 19 | 3.44 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 14 | 3.44 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 13 | 3.44 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 8 | 3.43 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 17 | 3.43 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 2 | 3.42 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 4 | 3.42 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 20 | 3.41 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 9 | 3.41 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 19 | 3.41 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 2 | 3.4 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 9 | 3.4 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 5 | 3.39 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 8 | 3.39 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 15 | 3.39 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 20 | 3.39 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 13 | 3.39 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 4 | 3.38 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 6 | 3.38 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 16 | 3.37 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 3 | 3.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 12 | 3.37 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 18 | 3.37 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 5 | 3.37 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 16 | 3.37 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 20 | 3.37 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 2 | 3.37 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 5 | 3.37 |
| (1,1705) | 1:83:A:LYS:HB3 | 1:93:A:TYR:HE2 | 17 | 3.36 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 16 | 3.36 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 10 | 3.36 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 11 | 3.35 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 3 | 3.35 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 11 | 3.35 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 9 | 3.34 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 12 | 3.34 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 6 | 3.34 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 4 | 3.33 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 17 | 3.33 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 18 | 3.33 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 11 | 3.32 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 1 | 3.32 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 6 | 3.32 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 13 | 3.32 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 14 | 3.32 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 15 | 3.32 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 20 | 3.32 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 10 | 3.31 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 2 | 3.31 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 8 | 3.31 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 14 | 3.31 |
| (1,585) | 1:25:A:SER:HB3 | 1:27:A:TYR:HE2 | 19 | 3.31 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 16 | 3.3 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 19 | 3.3 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 7 | 3.3 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 14 | 3.3 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 18 | 3.3 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 1 | 3.29 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 4 | 3.29 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 9 | 3.29 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 10 | 3.29 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 6 | 3.29 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 18 | 3.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 1 | 3.29 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 14 | 3.28 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 18 | 3.28 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 4 | 3.28 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 14 | 3.28 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 7 | 3.28 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 11 | 3.28 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 19 | 3.28 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 12 | 3.27 |
| (1,1318) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HB2 | 17 | 3.27 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 15 | 3.27 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 3 | 3.26 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 4 | 3.26 |
| (1,1158) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HE1 | 8 | 3.26 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 5 | 3.26 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 15 | 3.25 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 11 | 3.25 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 12 | 3.25 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 8 | 3.25 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 12 | 3.25 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 7 | 3.25 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 1 | 3.24 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 5 | 3.24 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 6 | 3.24 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 13 | 3.24 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 1 | 3.24 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 18 | 3.24 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 8 | 3.23 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 5 | 3.23 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 7 | 3.22 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 9 | 3.22 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 16 | 3.22 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 19 | 3.22 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 6 | 3.22 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 20 | 3.21 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 6 | 3.21 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 8 | 3.21 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 14 | 3.21 |
| (1,222) | 1:9:A:HIS:H | 1:27:A:TYR:HD2 | 3 | 3.21 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 10 | 3.2 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 3 | 3.2 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 9 | 3.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 15 | 3.2 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 2 | 3.2 |
| (1,619) | 1:27:A:TYR:HD1 | 1:32:A:PHE:HA | 4 | 3.2 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 11 | 3.2 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 12 | 3.2 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 16 | 3.2 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 2 | 3.19 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 10 | 3.19 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 13 | 3.19 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 2 | 3.19 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 3 | 3.19 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 5 | 3.19 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 13 | 3.19 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 17 | 3.19 |
| (1,1799) | 1:88:A:LEU:HG | 1:93:A:TYR:HD2 | 17 | 3.18 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 8 | 3.18 |
| (1,1159) | 1:56:A:TYR:HB2 | 1:66:A:PHE:HE1 | 3 | 3.18 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 11 | 3.18 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 8 | 3.18 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 19 | 3.17 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 15 | 3.17 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 20 | 3.17 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 10 | 3.17 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 2 | 3.16 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 7 | 3.16 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 8 | 3.16 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 5 | 3.16 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 18 | 3.16 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 20 | 3.16 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 14 | 3.16 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 20 | 3.15 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 12 | 3.15 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 13 | 3.15 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 14 | 3.15 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 17 | 3.15 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 10 | 3.15 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 6 | 3.14 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 9 | 3.14 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 10 | 3.14 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 2 | 3.14 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 7 | 3.14 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 15 | 3.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 11 | 3.14 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 17 | 3.13 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 12 | 3.13 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 17 | 3.13 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 13 | 3.13 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 15 | 3.13 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 9 | 3.13 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 17 | 3.13 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 4 | 3.12 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 2 | 3.12 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 20 | 3.12 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 4 | 3.12 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 19 | 3.12 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 16 | 3.12 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 20 | 3.12 |
| (1,1706) | 1:83:A:LYS:HB2 | 1:93:A:TYR:HD2 | 16 | 3.11 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 16 | 3.11 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 19 | 3.11 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 4 | 3.11 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 5 | 3.11 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 18 | 3.11 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 13 | 3.11 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 14 | 3.11 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 9 | 3.11 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 4 | 3.11 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 13 | 3.11 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 1 | 3.1 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 7 | 3.1 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 11 | 3.1 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 12 | 3.1 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 15 | 3.1 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 19 | 3.1 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 14 | 3.1 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 18 | 3.1 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 19 | 3.1 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 1 | 3.09 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 8 | 3.09 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 9 | 3.09 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 8 | 3.09 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 9 | 3.09 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 18 | 3.09 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 20 | 3.09 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 16 | 3.09 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 10 | 3.09 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 2 | 3.09 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 12 | 3.09 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 16 | 3.09 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 20 | 3.09 |
| (1,1321) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HA | 17 | 3.08 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 3 | 3.08 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 13 | 3.08 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 16 | 3.08 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 1 | 3.08 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 20 | 3.08 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 8 | 3.08 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 14 | 3.08 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 1 | 3.08 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 8 | 3.08 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 10 | 3.08 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 15 | 3.08 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 13 | 3.08 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 8 | 3.07 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 9 | 3.07 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 11 | 3.07 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 5 | 3.07 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 11 | 3.07 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 16 | 3.07 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 9 | 3.07 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 19 | 3.07 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 12 | 3.07 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 14 | 3.06 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 12 | 3.06 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 14 | 3.06 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 18 | 3.06 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 10 | 3.06 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 18 | 3.06 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 7 | 3.06 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 11 | 3.06 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 18 | 3.06 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 13 | 3.05 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 7 | 3.05 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 1 | 3.05 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 3 | 3.05 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 18 | 3.05 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 9 | 3.05 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 17 | 3.05 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 10 | 3.04 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 2 | 3.04 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 16 | 3.04 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 17 | 3.04 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 3 | 3.04 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 7 | 3.04 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 8 | 3.04 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 14 | 3.04 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 6 | 3.03 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 16 | 3.03 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 19 | 3.03 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 15 | 3.03 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 19 | 3.03 |
| (1,584) | 1:25:A:SER:HB3 | 1:27:A:TYR:HD2 | 19 | 3.03 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 3 | 3.03 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 5 | 3.03 |
| (1,368) | 1:15:A:PHE:HE2 | 1:29:A:VAL:H | 6 | 3.03 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 15 | 3.03 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 11 | 3.02 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 7 | 3.02 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 17 | 3.02 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 1 | 3.02 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 4 | 3.02 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 10 | 3.02 |
| (1,1320) | 1:66:A:PHE:HD2 | 1:75:A:LEU:H | 11 | 3.01 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 3 | 3.01 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 5 | 3.01 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 6 | 3.01 |
| (1,1250) | 1:61:A:TRP:HB3 | 1:66:A:PHE:HD1 | 20 | 3.0 |
| (1,1109) | 1:54:A:LEU:HB3 | 1:66:A:PHE:HD1 | 6 | 3.0 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 19 | 3.0 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 18 | 2.99 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 12 | 2.98 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 1 | 2.97 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 15 | 2.97 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 18 | 2.97 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 18 | 2.97 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 9 | 2.97 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 8 | 2.97 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 9 | 2.96 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 18 | 2.96 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 4 | 2.96 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 4 | 2.96 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 8 | 2.96 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 4 | 2.95 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 8 | 2.95 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 14 | 2.95 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 3 | 2.94 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 5 | 2.94 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 7 | 2.94 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 16 | 2.94 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 19 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 1 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 1 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 3 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 3 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 5 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 5 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 12 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 12 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 14 | 2.94 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 14 | 2.94 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 14 | 2.94 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 6 | 2.94 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 8 | 2.93 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 2 | 2.93 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 6 | 2.93 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 13 | 2.93 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 20 | 2.93 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 14 | 2.93 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 4 | 2.93 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 5 | 2.93 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 17 | 2.92 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 13 | 2.92 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 13 | 2.92 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 20 | 2.92 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 20 | 2.92 |
| (1,1784) | 1:88:A:LEU:HA | 1:93:A:TYR:HD2 | 10 | 2.91 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 8 | 2.91 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 8 | 2.91 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 6 | 2.91 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 11 | 2.91 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 2 | 2.91 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 19 | 2.9 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 19 | 2.9 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 17 | 2.9 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 18 | 2.9 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 14 | 2.9 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 12 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 2 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 2 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 9 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 9 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 10 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 10 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 15 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 15 | 2.89 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 12 | 2.89 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 18 | 2.89 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 9 | 2.89 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 13 | 2.89 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 6 | 2.88 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 6 | 2.88 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 11 | 2.88 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 11 | 2.88 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 17 | 2.88 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 17 | 2.88 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 5 | 2.88 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 20 | 2.88 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 15 | 2.88 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 5 | 2.87 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 1 | 2.87 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 10 | 2.87 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 12 | 2.87 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 16 | 2.87 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 17 | 2.87 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 20 | 2.87 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 18 | 2.86 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 16 | 2.86 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 16 | 2.86 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 9 | 2.86 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 16 | 2.86 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 2 | 2.86 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 4 | 2.86 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 8 | 2.86 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 9 | 2.86 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 11 | 2.86 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 18 | 2.86 |
| (1,1708) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HD2 | 7 | 2.85 |
| (1,1708) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HD2 | 7 | 2.85 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 1 | 2.85 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 7 | 2.85 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 19 | 2.85 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 1 | 2.85 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 2 | 2.84 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 5 | 2.84 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 2 | 2.84 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 13 | 2.84 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 15 | 2.84 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 4 | 2.83 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 6 | 2.83 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 4 | 2.83 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 11 | 2.83 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 16 | 2.83 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 3 | 2.83 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 2 | 2.82 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 1 | 2.82 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 3 | 2.82 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 14 | 2.82 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 17 | 2.82 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 3 | 2.82 |
| (1,543) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HD1 | 7 | 2.82 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 5 | 2.82 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 6 | 2.81 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 10 | 2.81 |
| (1,310) | 1:14:A:LEU:HA | 1:15:A:PHE:HE2 | 6 | 2.81 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 7 | 2.81 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 12 | 2.8 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 15 | 2.8 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 20 | 2.8 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 17 | 2.79 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 7 | 2.78 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 8 | 2.78 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 20 | 2.78 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 17 | 2.78 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 11 | 2.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 19 | 2.77 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 11 | 2.77 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 19 | 2.77 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 19 | 2.77 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 20 | 2.76 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 2 | 2.76 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 6 | 2.76 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 9 | 2.76 |
| (1,223) | 1:9:A:HIS:H | 1:27:A:TYR:HE2 | 3 | 2.76 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 7 | 2.75 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 16 | 2.75 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 2 | 2.75 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 8 | 2.74 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 19 | 2.74 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 7 | 2.74 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 17 | 2.74 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 10 | 2.73 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 5 | 2.73 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 12 | 2.73 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 18 | 2.72 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 12 | 2.72 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 14 | 2.72 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 10 | 2.72 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 13 | 2.72 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 19 | 2.71 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 2 | 2.71 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 6 | 2.71 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 7 | 2.71 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 5 | 2.71 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 4 | 2.71 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 10 | 2.71 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 5 | 2.71 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 5 | 2.71 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 20 | 2.7 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 4 | 2.7 |
| (1,1859) | 1:93:A:TYR:HD1 | 1:94:A:SER:HA | 13 | 2.7 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 8 | 2.7 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 8 | 2.7 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 13 | 2.7 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 15 | 2.7 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 19 | 2.7 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 13 | 2.69 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 7 | 2.69 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 9 | 2.69 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 4 | 2.68 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 15 | 2.68 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 17 | 2.68 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 11 | 2.68 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 15 | 2.68 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 4 | 2.68 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 12 | 2.68 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 5 | 2.67 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 9 | 2.67 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 10 | 2.67 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 12 | 2.67 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 4 | 2.67 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 11 | 2.67 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 3 | 2.67 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 20 | 2.67 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 15 | 2.67 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 1 | 2.66 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 1 | 2.66 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 7 | 2.66 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 10 | 2.66 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 12 | 2.66 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 18 | 2.66 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 3 | 2.65 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 14 | 2.65 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 10 | 2.65 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 6 | 2.65 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 2 | 2.64 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 16 | 2.64 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 17 | 2.64 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 18 | 2.64 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 19 | 2.64 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 8 | 2.64 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 15 | 2.64 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 6 | 2.64 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 15 | 2.63 |
| (1,1875) | 1:94:A:SER:HA | 1:97:A:TYR:HD1 | 14 | 2.63 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 9 | 2.63 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 20 | 2.63 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 1 | 2.63 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 5 | 2.63 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 6 | 2.63 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 5 | 2.63 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 1 | 2.62 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 4 | 2.62 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 13 | 2.62 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 14 | 2.62 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 17 | 2.62 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 16 | 2.62 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 4 | 2.61 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 13 | 2.6 |
| (1,1330) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB3 | 6 | 2.6 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 9 | 2.6 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 2 | 2.6 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 16 | 2.59 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 18 | 2.59 |
| (1,1108) | 1:54:A:LEU:HB2 | 1:66:A:PHE:HD1 | 1 | 2.59 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 15 | 2.59 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 9 | 2.58 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 13 | 2.58 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 12 | 2.58 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 5 | 2.58 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 6 | 2.58 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 10 | 2.57 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 19 | 2.57 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 3 | 2.56 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 2 | 2.55 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 20 | 2.55 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 1 | 2.55 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 3 | 2.55 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 2 | 2.54 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 4 | 2.54 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 7 | 2.54 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 8 | 2.54 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 19 | 2.54 |
| (1,1901) | 1:97:A:TYR:HD1 | 1:98:A:SER:HA | 14 | 2.53 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 10 | 2.53 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 9 | 2.53 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 11 | 2.53 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 17 | 2.53 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 18 | 2.53 |
| (1,1329) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HB2 | 6 | 2.52 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 13 | 2.52 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 3 | 2.52 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 19 | 2.52 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 10 | 2.52 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 12 | 2.52 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 15 | 2.52 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 1 | 2.51 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 7 | 2.51 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 9 | 2.51 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 1 | 2.51 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 16 | 2.51 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 20 | 2.51 |
| (1,544) | 1:22:A:ARG:HD3 | 1:27:A:TYR:HE1 | 3 | 2.5 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 7 | 2.5 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 13 | 2.5 |
| (1,357) | 1:15:A:PHE:HD1 | 1:16:A:GLY:HA3 | 14 | 2.5 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 2 | 2.49 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 11 | 2.49 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 16 | 2.48 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 4 | 2.48 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 17 | 2.47 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 18 | 2.47 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 17 | 2.46 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 20 | 2.46 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 7 | 2.46 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 8 | 2.46 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 10 | 2.46 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 4 | 2.45 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 9 | 2.45 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 20 | 2.45 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 20 | 2.45 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 1 | 2.44 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 3 | 2.44 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 10 | 2.44 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 13 | 2.44 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 15 | 2.44 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 15 | 2.44 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 18 | 2.43 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 19 | 2.43 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 16 | 2.43 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 13 | 2.43 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 18 | 2.42 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 7 | 2.42 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 13 | 2.42 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 11 | 2.42 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 12 | 2.42 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 12 | 2.42 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 17 | 2.42 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 19 | 2.41 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 16 | 2.41 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 20 | 2.41 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 20 | 2.41 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 12 | 2.4 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 18 | 2.4 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 1 | 2.4 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 14 | 2.4 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 16 | 2.4 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 1 | 2.39 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 11 | 2.38 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 14 | 2.38 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 12 | 2.38 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 14 | 2.37 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 17 | 2.37 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 2 | 2.37 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 8 | 2.37 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 17 | 2.37 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 8 | 2.37 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 10 | 2.37 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 15 | 2.37 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 18 | 2.37 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 1 | 2.36 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 3 | 2.36 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 11 | 2.36 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 14 | 2.36 |
| (1,587) | 1:25:A:SER:HB2 | 1:27:A:TYR:HE2 | 14 | 2.36 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 4 | 2.36 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 17 | 2.36 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 12 | 2.35 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 10 | 2.35 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 18 | 2.35 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 6 | 2.35 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 2 | 2.35 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 11 | 2.35 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 15 | 2.34 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 6 | 2.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 11 | 2.34 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 1 | 2.34 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 7 | 2.34 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 19 | 2.34 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 15 | 2.33 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 5 | 2.33 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 3 | 2.33 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 9 | 2.33 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 7 | 2.32 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 8 | 2.32 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 20 | 2.32 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 1 | 2.32 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 11 | 2.31 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 12 | 2.31 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 2 | 2.31 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 4 | 2.31 |
| (1,359) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB2 | 13 | 2.31 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 6 | 2.3 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 19 | 2.3 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 14 | 2.3 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 15 | 2.3 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 9 | 2.3 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 7 | 2.3 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 2 | 2.29 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 9 | 2.29 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 7 | 2.29 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 9 | 2.29 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 18 | 2.29 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 6 | 2.29 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 16 | 2.28 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 5 | 2.27 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 5 | 2.27 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 5 | 2.27 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 5 | 2.27 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 8 | 2.27 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 10 | 2.26 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 8 | 2.26 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 16 | 2.26 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 19 | 2.26 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 5 | 2.26 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 3 | 2.26 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 9 | 2.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 3 | 2.25 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 5 | 2.25 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 3 | 2.25 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 6 | 2.25 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 14 | 2.25 |
| (1,308) | 1:14:A:LEU:HB3 | 1:15:A:PHE:HD2 | 5 | 2.25 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 4 | 2.24 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 6 | 2.24 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 13 | 2.24 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 2 | 2.24 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 5 | 2.23 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 13 | 2.23 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 2 | 2.23 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 10 | 2.23 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 17 | 2.23 |
| (1,1798) | 1:88:A:LEU:H | 1:93:A:TYR:HD2 | 20 | 2.23 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 8 | 2.23 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 8 | 2.23 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 8 | 2.23 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 15 | 2.23 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 15 | 2.23 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 15 | 2.23 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 4 | 2.23 |
| (1,1864) | 1:93:A:TYR:HE1 | 1:94:A:SER:HA | 4 | 2.22 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 2 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 2 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 2 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 12 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 12 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 12 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 20 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 20 | 2.21 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 20 | 2.21 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 1 | 2.21 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 2 | 2.19 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 18 | 2.18 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 18 | 2.18 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 18 | 2.18 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 4 | 2.17 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 4 | 2.17 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 4 | 2.17 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 4 | 2.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 7 | 2.17 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 1 | 2.16 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 1 | 2.16 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 1 | 2.16 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 16 | 2.15 |
| (1,542) | 1:22:A:ARG:HG2 | 1:27:A:TYR:HE1 | 3 | 2.15 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 9 | 2.14 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 9 | 2.14 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 9 | 2.14 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 5 | 2.14 |
| (1,1161) | 1:56:A:TYR:HB3 | 1:66:A:PHE:HD1 | 8 | 2.13 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 19 | 2.12 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 13 | 2.12 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 13 | 2.12 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 13 | 2.12 |
| (1,556) | 1:22:A:ARG:HD2 | 1:36:A:PHE:HE1 | 6 | 2.11 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 14 | 2.11 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 14 | 2.11 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 14 | 2.11 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 16 | 2.1 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 16 | 2.1 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 16 | 2.1 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 20 | 2.1 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 20 | 2.1 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 20 | 2.1 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 18 | 2.09 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 18 | 2.09 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 12 | 2.09 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 12 | 2.09 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 12 | 2.09 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 15 | 2.09 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 15 | 2.09 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 15 | 2.09 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 13 | 2.09 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 13 | 2.09 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 13 | 2.09 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 4 | 2.08 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 4 | 2.08 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 4 | 2.08 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 1 | 2.08 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 1 | 2.08 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 1 | 2.08 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 8 | 2.08 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 8 | 2.08 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 8 | 2.08 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 18 | 2.08 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 18 | 2.08 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 18 | 2.08 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 14 | 2.08 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 14 | 2.08 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 14 | 2.08 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 5 | 2.07 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 5 | 2.07 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 5 | 2.07 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 12 | 2.07 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 15 | 2.07 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 10 | 2.07 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 10 | 2.07 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 10 | 2.07 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 11 | 2.07 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 11 | 2.07 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 11 | 2.07 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 17 | 2.07 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 17 | 2.07 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 17 | 2.07 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 16 | 2.07 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 16 | 2.07 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 16 | 2.07 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 20 | 2.07 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 20 | 2.07 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 20 | 2.07 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 12 | 2.06 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 12 | 2.06 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 12 | 2.06 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 4 | 2.06 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 4 | 2.06 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 12 | 2.06 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 12 | 2.06 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 3 | 2.06 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 9 | 2.06 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 9 | 2.06 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 9 | 2.06 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 12 | 2.06 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 12 | 2.06 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 12 | 2.06 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 15 | 2.06 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 15 | 2.06 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 15 | 2.06 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 14 | 2.05 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 14 | 2.05 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 3 | 2.05 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 3 | 2.05 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 3 | 2.05 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 5 | 2.05 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 2 | 2.05 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 2 | 2.05 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 2 | 2.05 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 4 | 2.05 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 4 | 2.05 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 4 | 2.05 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 19 | 2.05 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 19 | 2.05 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 19 | 2.05 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 1 | 2.05 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 1 | 2.05 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 1 | 2.05 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 8 | 2.05 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 8 | 2.05 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 8 | 2.05 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 10 | 2.05 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 10 | 2.05 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 10 | 2.05 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 11 | 2.05 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 11 | 2.05 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 11 | 2.05 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 17 | 2.05 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 17 | 2.05 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 17 | 2.05 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 18 | 2.05 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 18 | 2.05 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 18 | 2.05 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 8 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 8 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 8 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 9 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 9 | 2.04 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 9 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 18 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 18 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 18 | 2.04 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 1 | 2.04 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 1 | 2.04 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 7 | 2.04 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 3 | 2.04 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 3 | 2.04 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 3 | 2.04 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 9 | 2.04 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 9 | 2.04 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 9 | 2.04 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 1 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 1 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 1 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 6 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 6 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 6 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 11 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 11 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 11 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 13 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 13 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 13 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 20 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 20 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 20 | 2.03 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 6 | 2.03 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 6 | 2.03 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 6 | 2.03 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 14 | 2.03 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 14 | 2.03 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 14 | 2.03 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 1 | 2.03 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 7 | 2.03 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 7 | 2.03 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 7 | 2.03 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 2 | 2.03 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 2 | 2.03 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 2 | 2.03 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 3 | 2.03 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 3 | 2.03 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 3 | 2.03 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 4 | 2.03 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 4 | 2.03 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 4 | 2.03 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 19 | 2.03 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 19 | 2.03 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 19 | 2.03 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 2 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 2 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 2 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 14 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 14 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 14 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 15 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 15 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 15 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 19 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 19 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 19 | 2.02 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 3 | 2.02 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 3 | 2.02 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 5 | 2.02 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 5 | 2.02 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 10 | 2.02 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 10 | 2.02 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 10 | 2.02 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 13 | 2.02 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 13 | 2.02 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 13 | 2.02 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 2 | 2.02 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 6 | 2.02 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 7 | 2.02 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 7 | 2.02 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 7 | 2.02 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 7 | 2.01 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 7 | 2.01 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 7 | 2.01 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 10 | 2.01 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 10 | 2.01 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 10 | 2.01 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 16 | 2.01 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 16 | 2.01 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 16 | 2.01 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 19 | 2.01 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 19 | 2.01 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 19 | 2.01 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 13 | 2.01 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 8 | 2.01 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 3 | 2.0 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 3 | 2.0 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 3 | 2.0 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 8 | 2.0 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 8 | 2.0 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 7 | 2.0 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 7 | 2.0 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 7 | 2.0 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 8 | 2.0 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 11 | 2.0 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 12 | 2.0 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 15 | 2.0 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 10 | 2.0 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 9 | 2.0 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 18 | 2.0 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 19 | 2.0 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 6 | 2.0 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 6 | 2.0 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 6 | 2.0 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 6 | 2.0 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 6 | 2.0 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 6 | 2.0 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 19 | 1.99 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 19 | 1.99 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 20 | 1.99 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 20 | 1.99 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 16 | 1.99 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 4 | 1.99 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 6 | 1.99 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 10 | 1.99 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 16 | 1.99 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 16 | 1.98 |
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 16 | 1.98 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 16 | 1.98 |
| (1,1796) | 1:88:A:LEU:HD21 | 1:93:A:TYR:HD2 | 17 | 1.98 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1796) | 1:88:A:LEU:HD22 | 1:93:A:TYR:HD2 | 17 | 1.98 |
| (1,1796) | 1:88:A:LEU:HD23 | 1:93:A:TYR:HD2 | 17 | 1.98 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 13 | 1.98 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 13 | 1.98 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 11 | 1.98 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 11 | 1.98 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 11 | 1.98 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD11 | 17 | 1.98 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD12 | 17 | 1.98 |
| (1,1319) | 1:66:A:PHE:HD2 | 1:75:A:LEU:HD13 | 17 | 1.98 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 2 | 1.98 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 5 | 1.98 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 4 | 1.98 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 12 | 1.98 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 17 | 1.98 |
| (1,307) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HE2 | 5 | 1.98 |
| (1,307) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HE2 | 5 | 1.98 |
| (1,307) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HE2 | 5 | 1.98 |
| (1,306) | 1:14:A:LEU:HD11 | 1:15:A:PHE:HD2 | 5 | 1.98 |
| (1,306) | 1:14:A:LEU:HD12 | 1:15:A:PHE:HD2 | 5 | 1.98 |
| (1,306) | 1:14:A:LEU:HD13 | 1:15:A:PHE:HD2 | 5 | 1.98 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 7 | 1.97 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 7 | 1.97 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 9 | 1.97 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 9 | 1.97 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 15 | 1.97 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 15 | 1.97 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 9 | 1.97 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 20 | 1.97 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 8 | 1.97 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 11 | 1.97 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 14 | 1.97 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 15 | 1.97 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 5 | 1.96 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 16 | 1.96 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 3 | 1.96 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 20 | 1.96 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 10 | 1.95 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 10 | 1.95 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 11 | 1.95 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 11 | 1.95 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 3 | 1.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 3 | 1.95 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 3 | 1.95 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 17 | 1.95 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 7 | 1.95 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 13 | 1.95 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 2 | 1.94 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 2 | 1.94 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 14 | 1.94 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 14 | 1.94 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 17 | 1.93 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 7 | 1.93 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 7 | 1.93 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 7 | 1.93 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 8 | 1.93 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 8 | 1.93 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 6 | 1.92 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 6 | 1.92 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 16 | 1.92 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 16 | 1.92 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 1 | 1.92 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 2 | 1.92 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 4 | 1.92 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 1 | 1.92 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 15 | 1.92 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 15 | 1.92 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 15 | 1.92 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 9 | 1.92 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 11 | 1.92 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 20 | 1.92 |
| (1,369) | 1:15:A:PHE:HE2 | 1:30:A:VAL:H | 1 | 1.92 |
| (1,1709) | 1:83:A:LYS:HD2 | 1:93:A:TYR:HE2 | 17 | 1.91 |
| (1,1709) | 1:83:A:LYS:HD3 | 1:93:A:TYR:HE2 | 17 | 1.91 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 14 | 1.91 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 16 | 1.91 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 8 | 1.91 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 11 | 1.91 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 3 | 1.9 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 18 | 1.9 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 19 | 1.9 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 3 | 1.9 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 7 | 1.9 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 4 | 1.9 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 7 | 1.89 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 1 | 1.89 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 1 | 1.89 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 1 | 1.89 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 18 | 1.89 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 19 | 1.89 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 18 | 1.89 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 19 | 1.89 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 14 | 1.89 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 13 | 1.88 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 8 | 1.87 |
| (1,586) | 1:25:A:SER:HB2 | 1:27:A:TYR:HD2 | 14 | 1.87 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 9 | 1.87 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 19 | 1.87 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 15 | 1.86 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 13 | 1.86 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 13 | 1.86 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 13 | 1.86 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 14 | 1.86 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 16 | 1.86 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 2 | 1.85 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 4 | 1.85 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 12 | 1.85 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 15 | 1.85 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 20 | 1.85 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 10 | 1.85 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 11 | 1.85 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 18 | 1.85 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 18 | 1.85 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 5 | 1.84 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 8 | 1.84 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 9 | 1.84 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 11 | 1.84 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 18 | 1.84 |
| (1,1110) | 1:54:A:LEU:HG | 1:66:A:PHE:HD1 | 6 | 1.84 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 20 | 1.84 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 1 | 1.83 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 7 | 1.83 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 10 | 1.83 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 14 | 1.83 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 16 | 1.83 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 17 | 1.83 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 2 | 1.83 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 17 | 1.83 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 3 | 1.82 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 13 | 1.82 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 4 | 1.82 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 20 | 1.82 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 20 | 1.82 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 20 | 1.82 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 15 | 1.82 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 2 | 1.82 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 16 | 1.82 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 6 | 1.81 |
| (1,1315) | 1:66:A:PHE:HD2 | 1:67:A:HIS:H | 19 | 1.81 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 10 | 1.81 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 9 | 1.81 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 13 | 1.8 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 10 | 1.8 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 10 | 1.8 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 10 | 1.8 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 12 | 1.8 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 12 | 1.8 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 12 | 1.8 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 12 | 1.8 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 13 | 1.8 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 20 | 1.8 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 8 | 1.8 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 9 | 1.8 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 8 | 1.79 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 9 | 1.79 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 17 | 1.79 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 9 | 1.78 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 9 | 1.78 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 9 | 1.78 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 18 | 1.78 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 18 | 1.78 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 18 | 1.78 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 20 | 1.78 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 12 | 1.77 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 20 | 1.77 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 2 | 1.77 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 2 | 1.77 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 2 | 1.77 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 16 | 1.77 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 17 | 1.77 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 19 | 1.77 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 11 | 1.77 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 11 | 1.77 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 14 | 1.77 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 11 | 1.76 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 18 | 1.76 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 10 | 1.76 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 5 | 1.75 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 9 | 1.75 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 14 | 1.75 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 1 | 1.75 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 3 | 1.75 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 3 | 1.75 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 13 | 1.75 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 18 | 1.74 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 11 | 1.74 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 11 | 1.74 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 11 | 1.74 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 7 | 1.74 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 11 | 1.74 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 19 | 1.74 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 6 | 1.73 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 16 | 1.73 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 5 | 1.73 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 5 | 1.73 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 5 | 1.73 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 8 | 1.73 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 12 | 1.73 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 13 | 1.73 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 10 | 1.72 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 14 | 1.72 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 14 | 1.72 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 14 | 1.72 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 17 | 1.72 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 17 | 1.72 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 17 | 1.72 |
| (1,596) | 1:26:A:PRO:HA | 1:27:A:TYR:HD2 | 14 | 1.72 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 19 | 1.72 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 20 | 1.72 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 4 | 1.71 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 7 | 1.71 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 15 | 1.71 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 6 | 1.71 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 6 | 1.71 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 6 | 1.71 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 8 | 1.71 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 8 | 1.71 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 8 | 1.71 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 10 | 1.71 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 17 | 1.71 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 16 | 1.71 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 18 | 1.71 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 19 | 1.71 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 12 | 1.71 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 2 | 1.7 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 4 | 1.7 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 4 | 1.7 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 4 | 1.7 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 9 | 1.7 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 12 | 1.7 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 20 | 1.7 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 1 | 1.69 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 5 | 1.69 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 15 | 1.69 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 13 | 1.69 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 17 | 1.68 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 17 | 1.68 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 17 | 1.68 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 19 | 1.68 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 19 | 1.68 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 19 | 1.68 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 17 | 1.68 |
| (1,722) | 1:32:A:PHE:HA | 1:36:A:PHE:HE1 | 19 | 1.68 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 13 | 1.68 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 16 | 1.68 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 16 | 1.68 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 16 | 1.68 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 15 | 1.68 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 17 | 1.68 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 16 | 1.67 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 16 | 1.67 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 16 | 1.67 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 12 | 1.67 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 20 | 1.67 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 10 | 1.66 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 9 | 1.66 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 9 | 1.65 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 9 | 1.65 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 9 | 1.65 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 18 | 1.65 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 18 | 1.65 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 18 | 1.65 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 5 | 1.65 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 6 | 1.65 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 9 | 1.65 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 11 | 1.65 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 18 | 1.65 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 3 | 1.65 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 3 | 1.65 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 3 | 1.65 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 7 | 1.65 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 7 | 1.65 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 7 | 1.65 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 6 | 1.65 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 15 | 1.65 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 10 | 1.64 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 10 | 1.64 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 10 | 1.64 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 14 | 1.64 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 14 | 1.64 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 14 | 1.64 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 8 | 1.64 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 16 | 1.64 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 17 | 1.64 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 15 | 1.64 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 15 | 1.64 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 15 | 1.64 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 6 | 1.64 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 20 | 1.63 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 20 | 1.63 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 20 | 1.63 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 19 | 1.63 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 16 | 1.63 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 16 | 1.63 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 11 | 1.62 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 11 | 1.62 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 11 | 1.62 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 12 | 1.62 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 12 | 1.62 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 12 | 1.62 |
| (1,721) | 1:32:A:PHE:HA | 1:36:A:PHE:HD1 | 14 | 1.62 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD11 | 19 | 1.62 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD12 | 19 | 1.62 |
| (1,621) | 1:27:A:TYR:HD1 | 1:35:A:LEU:HD13 | 19 | 1.62 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 10 | 1.62 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 14 | 1.61 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 17 | 1.61 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 5 | 1.61 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 5 | 1.61 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 5 | 1.61 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 6 | 1.61 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 6 | 1.61 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 6 | 1.61 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 8 | 1.61 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 8 | 1.61 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 8 | 1.61 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 15 | 1.61 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 10 | 1.61 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 13 | 1.61 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 1 | 1.6 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 7 | 1.6 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 9 | 1.6 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 15 | 1.6 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 20 | 1.6 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 13 | 1.6 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 13 | 1.6 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 13 | 1.6 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 1 | 1.6 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 1 | 1.6 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 1 | 1.6 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 2 | 1.59 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 3 | 1.59 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 8 | 1.59 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 18 | 1.59 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 19 | 1.59 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 13 | 1.59 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 13 | 1.59 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 13 | 1.59 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 5 | 1.59 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 19 | 1.59 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 8 | 1.59 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 6 | 1.58 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 12 | 1.58 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 16 | 1.58 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 11 | 1.58 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 14 | 1.58 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 12 | 1.58 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 10 | 1.57 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 11 | 1.57 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 7 | 1.57 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 7 | 1.57 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 7 | 1.57 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 15 | 1.57 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 15 | 1.57 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 15 | 1.57 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 14 | 1.57 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 14 | 1.57 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 13 | 1.56 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 13 | 1.56 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 8 | 1.56 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 11 | 1.56 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 18 | 1.56 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 1 | 1.55 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 1 | 1.55 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 1 | 1.55 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 3 | 1.55 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 3 | 1.55 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 3 | 1.55 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 4 | 1.55 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 9 | 1.55 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 13 | 1.55 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 16 | 1.55 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 17 | 1.55 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 19 | 1.55 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 20 | 1.55 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 6 | 1.55 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 8 | 1.55 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 5 | 1.54 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 4 | 1.54 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 5 | 1.54 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 20 | 1.54 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 20 | 1.54 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 20 | 1.54 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 6 | 1.54 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 10 | 1.54 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 12 | 1.54 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 10 | 1.54 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 12 | 1.54 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 15 | 1.54 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 17 | 1.54 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 4 | 1.53 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 4 | 1.53 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 12 | 1.53 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 12 | 1.53 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 12 | 1.53 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 16 | 1.53 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 19 | 1.53 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 15 | 1.53 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 2 | 1.52 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 2 | 1.52 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 2 | 1.52 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 10 | 1.52 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 10 | 1.52 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 10 | 1.52 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 18 | 1.52 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 18 | 1.52 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 18 | 1.52 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 17 | 1.52 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 5 | 1.52 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 6 | 1.51 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 10 | 1.51 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 12 | 1.51 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 9 | 1.51 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 9 | 1.51 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 9 | 1.51 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 5 | 1.51 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 9 | 1.51 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 18 | 1.51 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 18 | 1.51 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 20 | 1.51 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 4 | 1.51 |
| (1,1863) | 1:93:A:TYR:HD1 | 1:94:A:SER:H | 13 | 1.5 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 2 | 1.5 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 3 | 1.5 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 9 | 1.5 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 16 | 1.5 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 19 | 1.5 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 4 | 1.5 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 4 | 1.5 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 4 | 1.5 |
| (1,791) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HE2 | 4 | 1.5 |
| (1,791) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HE2 | 4 | 1.5 |
| (1,791) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HE2 | 4 | 1.5 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 11 | 1.5 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 20 | 1.5 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 2 | 1.5 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 4 | 1.5 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 18 | 1.5 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 7 | 1.49 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 8 | 1.49 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 11 | 1.49 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 20 | 1.49 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 9 | 1.49 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 6 | 1.49 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 14 | 1.48 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 15 | 1.48 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 18 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 11 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 11 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 11 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 14 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 14 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 14 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 18 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 18 | 1.48 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 18 | 1.48 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 11 | 1.48 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 11 | 1.48 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 11 | 1.48 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 19 | 1.48 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 10 | 1.48 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 2 | 1.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 1 | 1.47 |
| (1,1849) | 1:93:A:TYR:HA | 1:93:A:TYR:HD2 | 17 | 1.47 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 5 | 1.47 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 5 | 1.47 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 5 | 1.47 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 14 | 1.47 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 14 | 1.47 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 14 | 1.47 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 2 | 1.47 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 9 | 1.47 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 5 | 1.47 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 3 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 3 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 3 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 6 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 6 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 6 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 12 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 12 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 12 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 13 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 13 | 1.46 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 13 | 1.46 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 17 | 1.45 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 17 | 1.45 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 17 | 1.45 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 3 | 1.45 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 13 | 1.45 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 8 | 1.44 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 8 | 1.44 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 8 | 1.44 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 8 | 1.44 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 8 | 1.44 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 8 | 1.44 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 14 | 1.44 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 16 | 1.44 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 1 | 1.44 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 7 | 1.44 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 2 | 1.44 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 4 | 1.44 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 14 | 1.44 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 20 | 1.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 1 | 1.43 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 1 | 1.43 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 1 | 1.43 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 15 | 1.43 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 15 | 1.43 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 15 | 1.43 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 16 | 1.43 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 4 | 1.43 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 5 | 1.43 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 6 | 1.43 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 16 | 1.43 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 9 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 9 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 9 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 19 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 19 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 19 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 20 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 20 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 20 | 1.42 |
| (1,614) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB3 | 8 | 1.42 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 2 | 1.42 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 1 | 1.42 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 10 | 1.42 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 12 | 1.42 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 15 | 1.42 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 17 | 1.42 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 12 | 1.42 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 13 | 1.42 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 8 | 1.42 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 7 | 1.41 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 7 | 1.41 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 7 | 1.41 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 10 | 1.41 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 10 | 1.41 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 10 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 2 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 2 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 2 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 5 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 5 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 5 | 1.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 16 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 16 | 1.41 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 16 | 1.41 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 2 | 1.41 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 4 | 1.41 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 2 | 1.41 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 4 | 1.41 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 8 | 1.41 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 9 | 1.41 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 11 | 1.41 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 18 | 1.41 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 11 | 1.41 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 17 | 1.41 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 2 | 1.4 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 2 | 1.4 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 2 | 1.4 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 16 | 1.4 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 16 | 1.4 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 16 | 1.4 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 12 | 1.4 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 6 | 1.4 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 6 | 1.4 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 6 | 1.4 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 5 | 1.4 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 6 | 1.4 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 11 | 1.4 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 7 | 1.4 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 19 | 1.4 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 14 | 1.4 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 19 | 1.4 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 4 | 1.39 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 4 | 1.39 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 4 | 1.39 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 1 | 1.39 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 7 | 1.39 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 12 | 1.39 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 3 | 1.39 |
| (1,1792) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HD2 | 17 | 1.38 |
| (1,1792) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HD2 | 17 | 1.38 |
| (1,1792) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HD2 | 17 | 1.38 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 20 | 1.38 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 16 | 1.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 5 | 1.37 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 17 | 1.37 |
| (1,601) | 1:27:A:TYR:HA | 1:27:A:TYR:HE2 | 3 | 1.37 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 10 | 1.37 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 7 | 1.36 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 8 | 1.36 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD11 | 19 | 1.36 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD12 | 19 | 1.36 |
| (1,620) | 1:27:A:TYR:HE1 | 1:35:A:LEU:HD13 | 19 | 1.36 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 3 | 1.36 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 17 | 1.36 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 5 | 1.36 |
| (1,349) | 1:15:A:PHE:HD2 | 1:15:A:PHE:H | 6 | 1.36 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 20 | 1.36 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 13 | 1.35 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 2 | 1.35 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 3 | 1.35 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 1 | 1.35 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 15 | 1.35 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 9 | 1.35 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 8 | 1.34 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 14 | 1.34 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 18 | 1.34 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 18 | 1.33 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 2 | 1.33 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 2 | 1.33 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 2 | 1.33 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 11 | 1.33 |
| (1,539) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HD1 | 7 | 1.33 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 13 | 1.33 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 15 | 1.33 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 13 | 1.32 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 20 | 1.32 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 14 | 1.31 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 10 | 1.31 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 12 | 1.31 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 15 | 1.31 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 10 | 1.3 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 17 | 1.3 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 17 | 1.3 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 17 | 1.3 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 20 | 1.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 20 | 1.3 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 20 | 1.3 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 16 | 1.3 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 18 | 1.3 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 19 | 1.3 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 9 | 1.3 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 13 | 1.3 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 20 | 1.3 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 8 | 1.3 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 11 | 1.3 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 14 | 1.3 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 18 | 1.3 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 10 | 1.3 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 6 | 1.3 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 1 | 1.3 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 12 | 1.29 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 4 | 1.29 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 6 | 1.29 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 12 | 1.29 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 12 | 1.29 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 12 | 1.29 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 20 | 1.29 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 16 | 1.29 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 17 | 1.29 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 19 | 1.29 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 16 | 1.29 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 17 | 1.29 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 18 | 1.29 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 19 | 1.29 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 20 | 1.29 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 4 | 1.29 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 5 | 1.29 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 11 | 1.28 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 11 | 1.28 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 11 | 1.28 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 9 | 1.28 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 17 | 1.28 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 11 | 1.28 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 18 | 1.28 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 9 | 1.28 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 13 | 1.28 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 1 | 1.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 3 | 1.28 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 5 | 1.28 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 12 | 1.28 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 18 | 1.27 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 9 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 4 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 4 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 4 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 5 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 5 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 5 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 14 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 14 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 14 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 15 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 15 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 15 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 16 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 16 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 16 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 19 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 19 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 19 | 1.27 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 19 | 1.27 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 19 | 1.27 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 19 | 1.27 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 8 | 1.27 |
| (1,607) | 1:27:A:TYR:HD2 | 1:27:A:TYR:H | 14 | 1.27 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 10 | 1.27 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 12 | 1.27 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 15 | 1.27 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 2 | 1.27 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 7 | 1.26 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 7 | 1.26 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 7 | 1.26 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 8 | 1.26 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 8 | 1.26 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 8 | 1.26 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 16 | 1.26 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 16 | 1.26 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 16 | 1.26 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 13 | 1.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 1 | 1.26 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 3 | 1.26 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 7 | 1.26 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 10 | 1.26 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 13 | 1.26 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 9 | 1.25 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 9 | 1.25 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 9 | 1.25 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 13 | 1.25 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 13 | 1.25 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 13 | 1.25 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 17 | 1.25 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 17 | 1.25 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 17 | 1.25 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 10 | 1.25 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 13 | 1.25 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 20 | 1.25 |
| (1,538) | 1:22:A:ARG:HB2 | 1:27:A:TYR:HE1 | 7 | 1.25 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 15 | 1.24 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 19 | 1.24 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 18 | 1.24 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 18 | 1.24 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 18 | 1.24 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 18 | 1.24 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 18 | 1.24 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 18 | 1.24 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 12 | 1.24 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 12 | 1.24 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 15 | 1.24 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 1 | 1.24 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 7 | 1.24 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 3 | 1.23 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 3 | 1.23 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 3 | 1.23 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 5 | 1.23 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 5 | 1.23 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 5 | 1.23 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 6 | 1.23 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 6 | 1.23 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 6 | 1.23 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 9 | 1.23 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 9 | 1.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 9 | 1.23 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 14 | 1.23 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 14 | 1.23 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 14 | 1.23 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 4 | 1.22 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 1 | 1.22 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 1 | 1.22 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 1 | 1.22 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 10 | 1.22 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 10 | 1.22 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 10 | 1.22 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 10 | 1.22 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 10 | 1.22 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 10 | 1.22 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 20 | 1.22 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 20 | 1.22 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 20 | 1.22 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 15 | 1.22 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 7 | 1.22 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 1 | 1.21 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 8 | 1.21 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 8 | 1.21 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 8 | 1.21 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 11 | 1.21 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 11 | 1.21 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 11 | 1.21 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 12 | 1.21 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 12 | 1.21 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 12 | 1.21 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 6 | 1.21 |
| (1,217) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HD2 | 3 | 1.21 |
| (1,1276) | 1:63:A:GLU:HA | 1:66:A:PHE:HD1 | 11 | 1.2 |
| (1,1113) | 1:54:A:LEU:HD11 | 1:66:A:PHE:HD1 | 6 | 1.2 |
| (1,1113) | 1:54:A:LEU:HD12 | 1:66:A:PHE:HD1 | 6 | 1.2 |
| (1,1113) | 1:54:A:LEU:HD13 | 1:66:A:PHE:HD1 | 6 | 1.2 |
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 17 | 1.2 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 6 | 1.2 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 4 | 1.2 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 15 | 1.2 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 13 | 1.19 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 13 | 1.19 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 13 | 1.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,555) | 1:22:A:ARG:HD3 | 1:36:A:PHE:HE1 | 11 | 1.19 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 3 | 1.19 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 5 | 1.19 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 2 | 1.18 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 4 | 1.18 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 5 | 1.18 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 6 | 1.18 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 2 | 1.18 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 7 | 1.17 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 7 | 1.17 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 7 | 1.17 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 15 | 1.17 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 15 | 1.17 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 15 | 1.17 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 6 | 1.17 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 1 | 1.16 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 1 | 1.16 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 1 | 1.16 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 2 | 1.16 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 2 | 1.16 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 2 | 1.16 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 3 | 1.16 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 3 | 1.16 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 3 | 1.16 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 3 | 1.16 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 7 | 1.16 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 4 | 1.16 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 5 | 1.16 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 4 | 1.16 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 1 | 1.15 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 6 | 1.15 |
| (1,790) | 1:35:A:LEU:HD21 | 1:36:A:PHE:HD2 | 4 | 1.14 |
| (1,790) | 1:35:A:LEU:HD22 | 1:36:A:PHE:HD2 | 4 | 1.14 |
| (1,790) | 1:35:A:LEU:HD23 | 1:36:A:PHE:HD2 | 4 | 1.14 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 7 | 1.14 |
| (1,540) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HE1 | 2 | 1.14 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 1 | 1.13 |
| (1,600) | 1:27:A:TYR:HA | 1:27:A:TYR:HD2 | 3 | 1.13 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 1 | 1.13 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 2 | 1.13 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 5 | 1.13 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 15 | 1.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 3 | 1.08 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 7 | 1.08 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 1 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 2 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 4 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 5 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 6 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 7 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 8 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 9 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 10 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 11 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 12 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 13 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 14 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 15 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 16 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 17 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 18 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 19 | 1.07 |
| (1,346) | 1:15:A:PHE:HB2 | 1:15:A:PHE:HD1 | 20 | 1.07 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 13 | 1.06 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 3 | 1.06 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 2 | 1.06 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 12 | 1.05 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 12 | 1.05 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 13 | 1.05 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 7 | 1.05 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 5 | 1.05 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 16 | 1.05 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 10 | 1.04 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 12 | 1.04 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 17 | 1.04 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 4 | 1.04 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 8 | 1.04 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 14 | 1.04 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 1 | 1.04 |
| (1,219) | 1:9:A:HIS:HB3 | 1:27:A:TYR:HE2 | 3 | 1.04 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 5 | 1.03 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 18 | 1.03 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 19 | 1.03 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 9 | 1.02 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 11 | 1.02 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 1 | 1.02 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 6 | 1.02 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 4 | 1.01 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 6 | 1.01 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 19 | 1.01 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 1 | 1.0 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 14 | 1.0 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 20 | 1.0 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 2 | 1.0 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 5 | 0.99 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 5 | 0.99 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 3 | 0.99 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 4 | 0.99 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 8 | 0.99 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 19 | 0.99 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 18 | 0.98 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 18 | 0.98 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 5 | 0.98 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 14 | 0.98 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 18 | 0.98 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 3 | 0.98 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 7 | 0.98 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 1 | 0.98 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 10 | 0.97 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 7 | 0.97 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 4 | 0.96 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 8 | 0.96 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 16 | 0.96 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 6 | 0.96 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 14 | 0.96 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 1 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 2 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 3 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 5 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 6 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 7 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 9 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 10 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 11 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 12 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 13 | 0.95 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 14 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 15 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 16 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 17 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 18 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 19 | 0.95 |
| (1,1307) | 1:66:A:PHE:HB2 | 1:66:A:PHE:HD1 | 20 | 0.95 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 8 | 0.95 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 9 | 0.95 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 9 | 0.95 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 11 | 0.95 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 5 | 0.93 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 1 | 0.93 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 12 | 0.93 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 15 | 0.93 |
| (1,220) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HE2 | 3 | 0.93 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 11 | 0.92 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 4 | 0.92 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 16 | 0.92 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 7 | 0.92 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 13 | 0.91 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 13 | 0.91 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 15 | 0.91 |
| (1,616) | 1:27:A:TYR:HE1 | 1:31:A:CYS:HB3 | 2 | 0.91 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 7 | 0.91 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 17 | 0.91 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 18 | 0.91 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 12 | 0.9 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 18 | 0.9 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 8 | 0.9 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 3 | 0.89 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 3 | 0.89 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 18 | 0.89 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 15 | 0.89 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 20 | 0.89 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 11 | 0.89 |
| (1,218) | 1:9:A:HIS:HB2 | 1:27:A:TYR:HD2 | 3 | 0.89 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 17 | 0.88 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 2 | 0.88 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 16 | 0.88 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 1 | 0.88 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 1 | 0.87 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 7 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 8 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 14 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 15 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 18 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 19 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 20 | 0.87 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 10 | 0.87 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 17 | 0.87 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 19 | 0.87 |
| (1,613) | 1:27:A:TYR:HD2 | 1:28:A:CYS:H | 3 | 0.87 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 17 | 0.87 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 20 | 0.87 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 2 | 0.86 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 3 | 0.86 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 6 | 0.86 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 9 | 0.86 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 10 | 0.86 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 11 | 0.86 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 12 | 0.86 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 16 | 0.86 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 12 | 0.86 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 9 | 0.86 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 11 | 0.85 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 4 | 0.85 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 5 | 0.85 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 13 | 0.85 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 12 | 0.85 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 14 | 0.85 |
| (1,1854) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HD2 | 13 | 0.84 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 3 | 0.84 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 13 | 0.84 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 14 | 0.84 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 6 | 0.84 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 17 | 0.84 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 20 | 0.84 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 6 | 0.83 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 10 | 0.83 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 13 | 0.83 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 9 | 0.82 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 11 | 0.82 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 5 | 0.82 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 19 | 0.82 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 17 | 0.81 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 8 | 0.81 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 15 | 0.81 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 18 | 0.81 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 11 | 0.8 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 11 | 0.8 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 2 | 0.8 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 9 | 0.8 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 11 | 0.8 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 18 | 0.8 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 20 | 0.8 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 10 | 0.8 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 15 | 0.8 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 5 | 0.8 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 10 | 0.79 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 13 | 0.79 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 4 | 0.79 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 4 | 0.79 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 4 | 0.79 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 4 | 0.79 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 13 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 1 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 2 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 3 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 4 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 6 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 7 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 8 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 9 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 10 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 11 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 12 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 13 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 14 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 15 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 16 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 17 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 18 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 19 | 0.79 |
| (1,343) | 1:15:A:PHE:HB3 | 1:15:A:PHE:HD2 | 20 | 0.79 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 7 | 0.78 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 9 | 0.78 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 4 | 0.78 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 18 | 0.78 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 18 | 0.78 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 18 | 0.78 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 5 | 0.78 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 7 | 0.78 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 19 | 0.78 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 12 | 0.78 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 14 | 0.78 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 16 | 0.78 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 16 | 0.77 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 16 | 0.77 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 10 | 0.77 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 5 | 0.77 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 5 | 0.77 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 5 | 0.77 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 14 | 0.77 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 14 | 0.77 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 14 | 0.77 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 20 | 0.77 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 1 | 0.77 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 5 | 0.77 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 8 | 0.77 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 11 | 0.77 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 18 | 0.77 |
| (1,358) | 1:15:A:PHE:HD1 | 1:17:A:LYS:HB3 | 13 | 0.77 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 11 | 0.76 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 16 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 6 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 6 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 6 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 11 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 11 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 11 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 12 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 12 | 0.76 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 12 | 0.76 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 12 | 0.76 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 16 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 7 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 9 | 0.76 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 10 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 13 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 14 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 15 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 16 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 17 | 0.76 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 20 | 0.76 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 12 | 0.76 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 5 | 0.75 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 19 | 0.75 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 3 | 0.75 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 3 | 0.75 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 3 | 0.75 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 17 | 0.75 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 2 | 0.75 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 6 | 0.75 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 19 | 0.75 |
| (1,615) | 1:27:A:TYR:HD1 | 1:31:A:CYS:HB2 | 8 | 0.75 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 2 | 0.75 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 4 | 0.75 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 10 | 0.74 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 10 | 0.74 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 2 | 0.74 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 6 | 0.74 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 9 | 0.74 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 12 | 0.74 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 14 | 0.74 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 20 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 8 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 8 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 8 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 13 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 13 | 0.74 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 13 | 0.74 |
| (1,1304) | 1:66:A:PHE:HA | 1:66:A:PHE:HD2 | 3 | 0.74 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 10 | 0.74 |
| (1,536) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HD1 | 15 | 0.74 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 7 | 0.73 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 8 | 0.73 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 17 | 0.73 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 15 | 0.73 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 15 | 0.73 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 15 | 0.73 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 3 | 0.72 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 18 | 0.72 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 1 | 0.72 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 1 | 0.72 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 1 | 0.72 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 8 | 0.71 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 20 | 0.71 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 1 | 0.71 |
| (1,1825) | 1:90:A:THR:HA | 1:93:A:TYR:HD1 | 15 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 9 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 9 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 9 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 19 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 19 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 19 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 20 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 20 | 0.71 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 20 | 0.71 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 5 | 0.71 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 5 | 0.71 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 5 | 0.71 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 3 | 0.7 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 10 | 0.7 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 10 | 0.7 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 10 | 0.7 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 12 | 0.7 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 12 | 0.7 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 12 | 0.7 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 6 | 0.69 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 16 | 0.69 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 2 | 0.69 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 2 | 0.69 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 2 | 0.69 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 7 | 0.69 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 7 | 0.69 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 7 | 0.69 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 1 | 0.69 |
| (1,1328) | 1:66:A:PHE:HD2 | 1:76:A:VAL:HA | 4 | 0.69 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 5 | 0.68 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 13 | 0.68 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 4 | 0.68 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 4 | 0.68 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 4 | 0.68 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 10 | 0.68 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 10 | 0.68 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 10 | 0.68 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 4 | 0.67 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 8 | 0.67 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 8 | 0.67 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 8 | 0.67 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 2 | 0.66 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 6 | 0.66 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 10 | 0.66 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 16 | 0.66 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 16 | 0.66 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 16 | 0.66 |
| (1,1791) | 1:88:A:LEU:HD11 | 1:93:A:TYR:HE2 | 17 | 0.66 |
| (1,1791) | 1:88:A:LEU:HD12 | 1:93:A:TYR:HE2 | 17 | 0.66 |
| (1,1791) | 1:88:A:LEU:HD13 | 1:93:A:TYR:HE2 | 17 | 0.66 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 7 | 0.66 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 7 | 0.66 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 7 | 0.66 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 3 | 0.65 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 8 | 0.65 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 9 | 0.65 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 12 | 0.65 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 19 | 0.65 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 20 | 0.65 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 11 | 0.65 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 11 | 0.65 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 11 | 0.65 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 15 | 0.65 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 15 | 0.65 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 15 | 0.65 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 5 | 0.65 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 7 | 0.64 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 11 | 0.64 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 14 | 0.64 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 15 | 0.64 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 16 | 0.64 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 18 | 0.64 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 2 | 0.64 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 2 | 0.64 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 2 | 0.64 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 2 | 0.63 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 1 | 0.63 |
| (1,1850) | 1:93:A:TYR:HA | 1:93:A:TYR:HE2 | 17 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 1 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 1 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 1 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 3 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 3 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 3 | 0.63 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 14 | 0.61 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 14 | 0.61 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 14 | 0.61 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 18 | 0.61 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 18 | 0.61 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 18 | 0.61 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 17 | 0.6 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 17 | 0.6 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 17 | 0.6 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 20 | 0.6 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 20 | 0.6 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 20 | 0.6 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 6 | 0.6 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 9 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 9 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 9 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 16 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 16 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 16 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 19 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 19 | 0.59 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 19 | 0.59 |
| (1,1868) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB3 | 19 | 0.57 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 13 | 0.56 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 13 | 0.56 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 13 | 0.56 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 1 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 2 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 3 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 4 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 7 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 8 | 0.55 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 11 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 12 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 13 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 15 | 0.55 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 20 | 0.55 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 1 | 0.55 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 3 | 0.55 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD21 | 6 | 0.54 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD22 | 6 | 0.54 |
| (1,1338) | 1:66:A:PHE:HE2 | 1:87:A:LEU:HD23 | 6 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 5 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 6 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 9 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 10 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 14 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 16 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 17 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 18 | 0.54 |
| (1,800) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HD1 | 19 | 0.54 |
| (1,537) | 1:22:A:ARG:HB3 | 1:27:A:TYR:HE1 | 7 | 0.52 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 2 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 3 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 4 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 5 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 6 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 8 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 9 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 10 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 11 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 12 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 13 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 15 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 16 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 19 | 0.51 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 1 | 0.5 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 7 | 0.5 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 14 | 0.5 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 17 | 0.5 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 18 | 0.5 |
| (1,1852) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HE1 | 20 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 1 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 2 | 0.5 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 4 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 8 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 11 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 12 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 13 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 15 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 18 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 20 | 0.5 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 3 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 5 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 6 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 7 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 9 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 10 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 14 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 16 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 17 | 0.49 |
| (1,799) | 1:36:A:PHE:HB2 | 1:36:A:PHE:HE1 | 19 | 0.49 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 5 | 0.47 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 4 | 0.47 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 11 | 0.47 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 13 | 0.47 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 4 | 0.46 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 4 | 0.46 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 5 | 0.46 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 9 | 0.46 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 12 | 0.46 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 15 | 0.46 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 16 | 0.46 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 2 | 0.46 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 3 | 0.46 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 4 | 0.46 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 5 | 0.46 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 9 | 0.46 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 12 | 0.46 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 13 | 0.46 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 1 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 2 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 6 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 7 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 8 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 10 | 0.45 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 17 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 18 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 19 | 0.45 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 20 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 1 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 6 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 7 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 8 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 10 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 11 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 14 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 15 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 16 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 17 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 18 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 19 | 0.45 |
| (1,1851) | 1:93:A:TYR:HB3 | 1:93:A:TYR:HD1 | 20 | 0.45 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 1 | 0.45 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 14 | 0.45 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 19 | 0.45 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 20 | 0.45 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 1 | 0.44 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 4 | 0.44 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 9 | 0.44 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 10 | 0.44 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 13 | 0.44 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 15 | 0.44 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 3 | 0.44 |
| (1,1857) | 1:93:A:TYR:HD2 | 1:93:A:TYR:H | 14 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 2 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 4 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 5 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 6 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 7 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 8 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 9 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 10 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 11 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 12 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 13 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 15 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 16 | 0.44 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 17 | 0.44 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 18 | 0.44 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 2 | 0.43 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 5 | 0.43 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 6 | 0.43 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 8 | 0.43 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 14 | 0.43 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 19 | 0.43 |
| (1,1311) | 1:66:A:PHE:HD1 | 1:66:A:PHE:H | 3 | 0.43 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 7 | 0.42 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 18 | 0.42 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 20 | 0.42 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 13 | 0.42 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 13 | 0.42 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 13 | 0.42 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 12 | 0.41 |
| (1,1900) | 1:97:A:TYR:HB3 | 1:97:A:TYR:HD1 | 17 | 0.4 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 11 | 0.4 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 11 | 0.4 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 1 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 2 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 7 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 8 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 9 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 14 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 15 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 16 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 17 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 18 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 19 | 0.39 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 20 | 0.39 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 14 | 0.39 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 14 | 0.39 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 14 | 0.39 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 20 | 0.39 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 20 | 0.39 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 20 | 0.39 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 9 | 0.38 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 9 | 0.38 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 3 | 0.38 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 4 | 0.38 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 6 | 0.38 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 10 | 0.38 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 11 | 0.38 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 12 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 1 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 1 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 1 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 4 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 4 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 4 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 16 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 16 | 0.38 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 16 | 0.38 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 19 | 0.37 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 19 | 0.37 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 5 | 0.37 |
| (1,1855) | 1:93:A:TYR:HB2 | 1:93:A:TYR:HE2 | 13 | 0.37 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 12 | 0.37 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 12 | 0.37 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 7 | 0.37 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 8 | 0.37 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 8 | 0.37 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 11 | 0.37 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 11 | 0.37 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 14 | 0.37 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 14 | 0.37 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 16 | 0.37 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 16 | 0.37 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 18 | 0.37 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 18 | 0.37 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 19 | 0.37 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 19 | 0.37 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 20 | 0.37 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 20 | 0.37 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 12 | 0.37 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 12 | 0.37 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 12 | 0.37 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 2 | 0.37 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 19 | 0.37 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 1 | 0.36 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 1 | 0.36 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 4 | 0.36 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 4 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 15 | 0.36 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 15 | 0.36 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 18 | 0.36 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 18 | 0.36 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 9 | 0.36 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 9 | 0.36 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 10 | 0.36 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 10 | 0.36 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 12 | 0.36 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 12 | 0.36 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 13 | 0.36 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 13 | 0.36 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 15 | 0.36 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 15 | 0.36 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 17 | 0.36 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 17 | 0.36 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 10 | 0.36 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 10 | 0.36 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 10 | 0.36 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 15 | 0.36 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 15 | 0.36 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 15 | 0.36 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 17 | 0.35 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 5 | 0.35 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 5 | 0.35 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 9 | 0.35 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 9 | 0.35 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 14 | 0.35 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 14 | 0.35 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 9 | 0.35 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 14 | 0.35 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 2 | 0.35 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 2 | 0.35 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 2 | 0.35 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 3 | 0.35 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 7 | 0.35 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 7 | 0.34 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 12 | 0.34 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 14 | 0.34 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 3 | 0.34 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 3 | 0.34 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 8 | 0.34 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 8 | 0.34 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 8 | 0.34 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 16 | 0.34 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 18 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 8 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 8 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 8 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 11 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 11 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 11 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 18 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 18 | 0.34 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 18 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 1 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 2 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 3 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 4 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 5 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 6 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 7 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 8 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 9 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 10 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 11 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 12 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 13 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 14 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 15 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 16 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 17 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 18 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 19 | 0.34 |
| (1,341) | 1:15:A:PHE:HA | 1:15:A:PHE:HD2 | 20 | 0.34 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 18 | 0.33 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 20 | 0.33 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 6 | 0.33 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 6 | 0.33 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 7 | 0.33 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 7 | 0.33 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 13 | 0.33 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 13 | 0.33 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 19 | 0.33 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 19 | 0.33 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 12 | 0.33 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 20 | 0.33 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 7 | 0.33 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 7 | 0.33 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 7 | 0.33 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 17 | 0.33 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 17 | 0.33 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 17 | 0.33 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 9 | 0.33 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 2 | 0.32 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 19 | 0.32 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 2 | 0.32 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 2 | 0.32 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 16 | 0.32 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 16 | 0.32 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 20 | 0.32 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 20 | 0.32 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 1 | 0.32 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 3 | 0.32 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 5 | 0.32 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 11 | 0.32 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 13 | 0.32 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 19 | 0.32 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 9 | 0.32 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 9 | 0.32 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 9 | 0.32 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 19 | 0.32 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 19 | 0.32 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 19 | 0.32 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 4 | 0.32 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 10 | 0.32 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 11 | 0.32 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 5 | 0.31 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 6 | 0.31 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 8 | 0.31 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 14 | 0.31 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 10 | 0.31 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 10 | 0.31 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 6 | 0.31 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 10 | 0.31 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 15 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 17 | 0.31 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 4 | 0.31 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 4 | 0.31 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 5 | 0.31 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 5 | 0.31 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 6 | 0.31 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 6 | 0.31 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 9 | 0.3 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 13 | 0.3 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 1 | 0.3 |
| (1,1788) | 1:88:A:LEU:HB2 | 1:93:A:TYR:HD2 | 17 | 0.3 |
| (1,1788) | 1:88:A:LEU:HB3 | 1:93:A:TYR:HD2 | 17 | 0.3 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 2 | 0.3 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 2 | 0.3 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 18 | 0.3 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 7 | 0.29 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 7 | 0.29 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 15 | 0.29 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 15 | 0.29 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 3 | 0.29 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 3 | 0.29 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 3 | 0.29 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 8 | 0.29 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 15 | 0.29 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 1 | 0.28 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 4 | 0.28 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 10 | 0.28 |
| (1,1899) | 1:97:A:TYR:HB2 | 1:97:A:TYR:HD2 | 15 | 0.28 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 2 | 0.28 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 2 | 0.28 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 1 | 0.28 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 1 | 0.28 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 3 | 0.28 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 3 | 0.28 |
| (1,603) | 1:27:A:TYR:HB2 | 1:27:A:TYR:HD1 | 7 | 0.28 |
| (1,603) | 1:27:A:TYR:HB3 | 1:27:A:TYR:HD1 | 7 | 0.28 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 12 | 0.28 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 11 | 0.27 |
| (1,518) | 1:22:A:ARG:HA | 1:22:A:ARG:HG3 | 2 | 0.27 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 17 | 0.27 |
| (1,1203) | 1:59:A:ARG:HG2 | 1:59:A:ARG:HE | 2 | 0.26 |
| (1,1203) | 1:59:A:ARG:HG2 | 1:59:A:ARG:HE | 7 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1203) | 1:59:A:ARG:HG2 | 1:59:A:ARG:HE | 18 | 0.26 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 2 | 0.26 |
| (1,518) | 1:22:A:ARG:HA | 1:22:A:ARG:HG3 | 4 | 0.26 |
| (1,518) | 1:22:A:ARG:HA | 1:22:A:ARG:HG3 | 5 | 0.26 |
| (1,518) | 1:22:A:ARG:HA | 1:22:A:ARG:HG3 | 6 | 0.26 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 6 | 0.26 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 6 | 0.26 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 6 | 0.26 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 16 | 0.26 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 1 | 0.26 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 13 | 0.26 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 16 | 0.26 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 20 | 0.26 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 6 | 0.25 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 6 | 0.25 |
| (1,1203) | 1:59:A:ARG:HG2 | 1:59:A:ARG:HE | 4 | 0.25 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 8 | 0.25 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 10 | 0.25 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 12 | 0.25 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 14 | 0.25 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 15 | 0.25 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 18 | 0.25 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 18 | 0.24 |
| (1,1044) | 1:52:A:LYS:HA | 1:52:A:LYS:HG3 | 3 | 0.24 |
| (1,1044) | 1:52:A:LYS:HA | 1:52:A:LYS:HG3 | 18 | 0.24 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 3 | 0.24 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG21 | 5 | 0.24 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG22 | 5 | 0.24 |
| (1,367) | 1:15:A:PHE:HE2 | 1:29:A:VAL:HG23 | 5 | 0.24 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 1 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 2 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 3 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 4 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 7 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 9 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 11 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 17 | 0.24 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 19 | 0.24 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 16 | 0.23 |
| (1,1044) | 1:52:A:LYS:HA | 1:52:A:LYS:HG3 | 10 | 0.23 |
| (1,806) | 1:36:A:PHE:HD2 | 1:36:A:PHE:H | 4 | 0.23 |
| (1,738) | 1:33:A:GLU:HG2 | 1:34:A:THR:H | 3 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 20 | 0.23 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 6 | 0.23 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 11 | 0.23 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 15 | 0.22 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 2 | 0.22 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 5 | 0.22 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 18 | 0.22 |
| (1,738) | 1:33:A:GLU:HG2 | 1:34:A:THR:H | 1 | 0.22 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 6 | 0.22 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 10 | 0.22 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 17 | 0.22 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 12 | 0.22 |
| (1,305) | 1:14:A:LEU:HG | 1:15:A:PHE:H | 5 | 0.22 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 1 | 0.22 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 2 | 0.22 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 4 | 0.22 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 7 | 0.22 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 8 | 0.21 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 18 | 0.21 |
| (1,1203) | 1:59:A:ARG:HG2 | 1:59:A:ARG:HE | 8 | 0.21 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 20 | 0.21 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 6 | 0.21 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 8 | 0.21 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 16 | 0.21 |
| (1,738) | 1:33:A:GLU:HG2 | 1:34:A:THR:H | 4 | 0.21 |
| (1,738) | 1:33:A:GLU:HG2 | 1:34:A:THR:H | 6 | 0.21 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 19 | 0.21 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 1 | 0.21 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 9 | 0.21 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 18 | 0.21 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 19 | 0.21 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 1 | 0.21 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 10 | 0.21 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 13 | 0.21 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 15 | 0.21 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 20 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 1 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 3 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 4 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 6 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 8 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 11 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 16 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 18 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 19 | 0.21 |
| (1,256) | 1:11:A:ASN:HA | 1:11:A:ASN:HB3 | 20 | 0.21 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 5 | 0.21 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 6 | 0.21 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 10 | 0.21 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 17 | 0.2 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 1 | 0.2 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 2 | 0.2 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 17 | 0.2 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 20 | 0.2 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 20 | 0.2 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 1 | 0.2 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 19 | 0.2 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 4 | 0.2 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 7 | 0.2 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 9 | 0.2 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 11 | 0.2 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 12 | 0.2 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 14 | 0.2 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 15 | 0.2 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 5 | 0.2 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 10 | 0.2 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 11 | 0.2 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 16 | 0.2 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 17 | 0.2 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 18 | 0.2 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 7 | 0.2 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 16 | 0.2 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 7 | 0.2 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 11 | 0.2 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 17 | 0.2 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 14 | 0.2 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 3 | 0.2 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 8 | 0.2 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 12 | 0.2 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 3 | 0.19 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 7 | 0.19 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 9 | 0.19 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 11 | 0.19 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 15 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 16 | 0.19 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 10 | 0.19 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 14 | 0.19 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 2 | 0.19 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 6 | 0.19 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 12 | 0.19 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 20 | 0.19 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 1 | 0.19 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 5 | 0.19 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 7 | 0.19 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 4 | 0.19 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 5 | 0.19 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 1 | 0.19 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 13 | 0.19 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 17 | 0.19 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 19 | 0.19 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 20 | 0.19 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 2 | 0.19 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 7 | 0.19 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 8 | 0.19 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 9 | 0.19 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 12 | 0.19 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 13 | 0.19 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 14 | 0.19 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 4 | 0.19 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 12 | 0.19 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 13 | 0.19 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 1 | 0.19 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 11 | 0.19 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 12 | 0.19 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 13 | 0.19 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 14 | 0.19 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 20 | 0.19 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 1 | 0.19 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 1 | 0.18 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 1 | 0.18 |
| (1,1867) | 1:93:A:TYR:HE1 | 1:97:A:TYR:HB2 | 7 | 0.18 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 4 | 0.18 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 10 | 0.18 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 12 | 0.18 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 13 | 0.18 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 14 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 19 | 0.18 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 4 | 0.18 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 12 | 0.18 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 14 | 0.18 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 19 | 0.18 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 17 | 0.18 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 1 | 0.18 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 4 | 0.18 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 5 | 0.18 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 15 | 0.18 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 18 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 2 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 3 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 9 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 10 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 11 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 12 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 16 | 0.18 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 17 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 1 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 2 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 3 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 4 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 5 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 6 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 7 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 8 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 9 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 10 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 11 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 12 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 13 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 14 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 15 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 16 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 17 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 18 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 19 | 0.18 |
| (1,1443) | 1:70:A:GLN:HG2 | 1:70:A:GLN:HE22 | 20 | 0.18 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 9 | 0.18 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 15 | 0.18 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 16 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 10 | 0.18 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 7 | 0.18 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 15 | 0.18 |
| (1,727) | 1:33:A:GLU:HA | 1:33:A:GLU:HG3 | 20 | 0.18 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 5 | 0.18 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 11 | 0.18 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 15 | 0.18 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 20 | 0.18 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 3 | 0.18 |
| (1,520) | 1:22:A:ARG:HA | 1:22:A:ARG:HD3 | 18 | 0.18 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 3 | 0.18 |
| (1,382) | 1:17:A:LYS:HG2 | 1:18:A:LYS:HA | 6 | 0.18 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 11 | 0.18 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 18 | 0.18 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 9 | 0.18 |
| (1,1897) | 1:97:A:TYR:HB2 | 1:98:A:SER:H | 12 | 0.17 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 5 | 0.17 |
| (1,1614) | 1:80:A:PHE:HB2 | 1:82:A:ALA:H | 6 | 0.17 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 13 | 0.17 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 16 | 0.17 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 9 | 0.17 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 17 | 0.17 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 6 | 0.17 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 13 | 0.17 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 15 | 0.17 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 18 | 0.17 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 19 | 0.17 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 20 | 0.17 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 1 | 0.17 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 11 | 0.17 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 15 | 0.17 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 6 | 0.17 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 8 | 0.17 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 12 | 0.17 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 18 | 0.17 |
| (1,983) | 1:46:A:PRO:HB2 | 1:46:A:PRO:HD2 | 3 | 0.17 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 19 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 1 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 3 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 8 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 11 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 13 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 14 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 15 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 18 | 0.17 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 20 | 0.17 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 8 | 0.17 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 14 | 0.17 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 7 | 0.17 |
| (1,394) | 1:18:A:LYS:HG3 | 1:18:A:LYS:H | 17 | 0.17 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 8 | 0.17 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 16 | 0.17 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 16 | 0.17 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 17 | 0.17 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 19 | 0.17 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 9 | 0.17 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 15 | 0.17 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 20 | 0.17 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 9 | 0.17 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 17 | 0.17 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 18 | 0.17 |
| (1,1897) | 1:97:A:TYR:HB2 | 1:98:A:SER:H | 18 | 0.16 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 19 | 0.16 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 5 | 0.16 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 2 | 0.16 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 6 | 0.16 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 7 | 0.16 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 2 | 0.16 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 3 | 0.16 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 7 | 0.16 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 10 | 0.16 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 13 | 0.16 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 14 | 0.16 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 16 | 0.16 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 19 | 0.16 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 4 | 0.16 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 14 | 0.16 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 14 | 0.16 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 16 | 0.16 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 17 | 0.16 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 2 | 0.16 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 1 | 0.16 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 4 | 0.16 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 2 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 5 | 0.16 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 9 | 0.16 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 10 | 0.16 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 12 | 0.16 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 16 | 0.16 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 17 | 0.16 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 19 | 0.16 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 6 | 0.16 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 6 | 0.16 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 15 | 0.16 |
| (1,190) | 1:8:A:HIS:HB3 | 1:26:A:PRO:HD2 | 18 | 0.16 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 3 | 0.16 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 8 | 0.16 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 10 | 0.16 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 13 | 0.16 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 16 | 0.16 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 18 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 8 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 10 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 11 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 14 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 16 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 19 | 0.16 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 20 | 0.16 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 1 | 0.16 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 20 | 0.15 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 20 | 0.15 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 5 | 0.15 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 4 | 0.15 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 7 | 0.15 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 12 | 0.15 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 14 | 0.15 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 17 | 0.15 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 18 | 0.15 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 3 | 0.15 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 17 | 0.15 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 20 | 0.15 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 1 | 0.15 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 6 | 0.15 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 8 | 0.15 |
| (1,1450) | 1:70:A:GLN:HG2 | 1:71:A:CYS:H | 8 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 3 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 6 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 10 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 13 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 14 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 15 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 16 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 17 | 0.15 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 19 | 0.15 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 5 | 0.15 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 3 | 0.15 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 7 | 0.15 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 11 | 0.15 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 14 | 0.15 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 17 | 0.15 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 7 | 0.15 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 13 | 0.15 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 14 | 0.15 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 16 | 0.15 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 20 | 0.15 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 4 | 0.15 |
| (1,797) | 1:36:A:PHE:HB3 | 1:36:A:PHE:H | 6 | 0.15 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 5 | 0.15 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 16 | 0.15 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 1 | 0.15 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 5 | 0.15 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 2 | 0.15 |
| (1,360) | 1:15:A:PHE:HE1 | 1:17:A:LYS:HB3 | 13 | 0.15 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 5 | 0.15 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 5 | 0.15 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 6 | 0.15 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 7 | 0.15 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 12 | 0.15 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 14 | 0.15 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 12 | 0.15 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 13 | 0.15 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 15 | 0.15 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 5 | 0.15 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 4 | 0.14 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 12 | 0.14 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 13 | 0.14 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 6 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 13 | 0.14 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 15 | 0.14 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 19 | 0.14 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 20 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 4 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 5 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 6 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 7 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 9 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 10 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 11 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 12 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 13 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 14 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 18 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 19 | 0.14 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 20 | 0.14 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 3 | 0.14 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 6 | 0.14 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 13 | 0.14 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 15 | 0.14 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 16 | 0.14 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 8 | 0.14 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 8 | 0.14 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 9 | 0.14 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 15 | 0.14 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 4 | 0.14 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 12 | 0.14 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD21 | 5 | 0.14 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD22 | 5 | 0.14 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD23 | 5 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 1 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 5 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 7 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 8 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 9 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 11 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 18 | 0.14 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 20 | 0.14 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 9 | 0.14 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 10 | 0.14 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 19 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 1 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 4 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 5 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 6 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 8 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 13 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 15 | 0.14 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 19 | 0.14 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 13 | 0.14 |
| (1,1011) | 1:47:A:ILE:HG12 | 1:60:A:HIS:HB3 | 7 | 0.14 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 12 | 0.14 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 17 | 0.14 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 9 | 0.14 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 11 | 0.14 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 1 | 0.14 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 6 | 0.14 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 9 | 0.14 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 13 | 0.14 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 15 | 0.14 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 18 | 0.14 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 20 | 0.14 |
| (1,750) | 1:33:A:GLU:HB3 | 1:49:A:CYS:H | 19 | 0.14 |
| (1,642) | 1:28:A:CYS:H | 1:32:A:PHE:H | 2 | 0.14 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 3 | 0.14 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 6 | 0.14 |
| (1,552) | 1:22:A:ARG:HD2 | 1:32:A:PHE:HD2 | 2 | 0.14 |
| (1,552) | 1:22:A:ARG:HD2 | 1:32:A:PHE:HD2 | 4 | 0.14 |
| (1,390) | 1:18:A:LYS:HA | 1:18:A:LYS:HG3 | 6 | 0.14 |
| (1,263) | 1:11:A:ASN:HB2 | 1:11:A:ASN:HD22 | 16 | 0.14 |
| (1,263) | 1:11:A:ASN:HB2 | 1:11:A:ASN:HD22 | 18 | 0.14 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 3 | 0.14 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 4 | 0.14 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 11 | 0.14 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 17 | 0.14 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 19 | 0.14 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 2 | 0.14 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 13 | 0.14 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 15 | 0.14 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 1 | 0.14 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 10 | 0.14 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 11 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|---------------|----------|---------------|
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 12 | 0.14 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 14 | 0.14 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 18 | 0.14 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 19 | 0.14 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 9 | 0.14 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 18 | 0.14 |
| (1,1897) | 1:97:A:TYR:HB2 | 1:98:A:SER:H | 5 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 1 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 2 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 6 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 11 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 13 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 14 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 15 | 0.13 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 19 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 2 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 3 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 6 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 8 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 9 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 10 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 15 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 16 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 17 | 0.13 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 18 | 0.13 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 9 | 0.13 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 8 | 0.13 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 16 | 0.13 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 1 | 0.13 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 3 | 0.13 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 8 | 0.13 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 15 | 0.13 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 16 | 0.13 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 17 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 7 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 9 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 10 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 11 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 14 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 17 | 0.13 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 18 | 0.13 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 1 | 0.13 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 5 | 0.13 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 11 | 0.13 |
| (1,1532) | 1:75:A:LEU:HB3 | 1:78:A:LYS:H | 18 | 0.13 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 4 | 0.13 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 5 | 0.13 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 7 | 0.13 |
| (1,1481) | 1:72:A:ARG:HA | 1:73:A:ASN:HB2 | 11 | 0.13 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 4 | 0.13 |
| (1,1308) | 1:66:A:PHE:HB3 | 1:66:A:PHE:HD2 | 12 | 0.13 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 2 | 0.13 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 6 | 0.13 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 8 | 0.13 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 2 | 0.13 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 9 | 0.13 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 11 | 0.13 |
| (1,1093) | 1:54:A:LEU:HG | 1:61:A:TRP:HB3 | 10 | 0.13 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 2 | 0.13 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 6 | 0.13 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 15 | 0.13 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 18 | 0.13 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 8 | 0.13 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 20 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 3 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 4 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 7 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 10 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 11 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 12 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 17 | 0.13 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 19 | 0.13 |
| (1,719) | 1:32:A:PHE:HA | 1:35:A:LEU:HG | 4 | 0.13 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 2 | 0.13 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 4 | 0.13 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 5 | 0.13 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 7 | 0.13 |
| (1,534) | 1:22:A:ARG:HA | 1:24:A:GLU:H | 12 | 0.13 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 2 | 0.13 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 4 | 0.13 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 10 | 0.13 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 12 | 0.13 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|--------------|----------|---------------|
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 2 | 0.13 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 4 | 0.13 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 10 | 0.13 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 11 | 0.13 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 16 | 0.13 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 19 | 0.13 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 20 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 1 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 1 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 1 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 2 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 2 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 2 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 3 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 3 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 3 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 4 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 4 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 4 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 5 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 5 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 5 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 7 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 7 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 7 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 8 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 8 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 8 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 9 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 9 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 9 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 10 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 10 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 10 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 11 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 11 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 11 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 12 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 12 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 12 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 13 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 13 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 14 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 14 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 14 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 16 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 16 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 16 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 17 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 17 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 17 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 19 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 19 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 19 | 0.13 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 20 | 0.13 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 20 | 0.13 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 20 | 0.13 |
| (1,263) | 1:11:A:ASN:HB2 | 1:11:A:ASN:HD22 | 8 | 0.13 |
| (1,263) | 1:11:A:ASN:HB2 | 1:11:A:ASN:HD22 | 11 | 0.13 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 1 | 0.13 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 6 | 0.13 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 20 | 0.13 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 2 | 0.13 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 5 | 0.13 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 9 | 0.13 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 10 | 0.13 |
| (1,182) | 1:8:A:HIS:HB2 | 1:25:A:SER:HA | 2 | 0.13 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 2 | 0.13 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 3 | 0.13 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 4 | 0.13 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 5 | 0.13 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 6 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 5 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 7 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 9 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 10 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 11 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 12 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 14 | 0.13 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 17 | 0.13 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 12 | 0.13 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 2 | 0.13 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 4 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 6 | 0.13 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 9 | 0.13 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 10 | 0.13 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 14 | 0.13 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 17 | 0.13 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 19 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 2 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 3 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 4 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 6 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 7 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 8 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 9 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 13 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 15 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 16 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 17 | 0.13 |
| (1,36) | 1:4:A:ARG:HB3 | 1:4:A:ARG:H | 20 | 0.13 |
| (1,1897) | 1:97:A:TYR:HB2 | 1:98:A:SER:H | 13 | 0.12 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 2 | 0.12 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 6 | 0.12 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 7 | 0.12 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 8 | 0.12 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 9 | 0.12 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 14 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 3 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 4 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 5 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 7 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 8 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 9 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 10 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 12 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 16 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 17 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 18 | 0.12 |
| (1,1829) | 1:91:A:ASP:HB2 | 1:91:A:ASP:HA | 20 | 0.12 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 1 | 0.12 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 7 | 0.12 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 14 | 0.12 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 20 | 0.12 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 2 | 0.12 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 11 | 0.12 |
| (1,1726) | 1:85:A:ASP:HB3 | 1:85:A:ASP:H | 2 | 0.12 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 1 | 0.12 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 4 | 0.12 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 5 | 0.12 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 8 | 0.12 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 12 | 0.12 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 19 | 0.12 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 20 | 0.12 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 4 | 0.12 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 5 | 0.12 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 9 | 0.12 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 12 | 0.12 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 18 | 0.12 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 12 | 0.12 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 9 | 0.12 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 2 | 0.12 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 3 | 0.12 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 18 | 0.12 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD21 | 12 | 0.12 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD22 | 12 | 0.12 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD23 | 12 | 0.12 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 20 | 0.12 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 10 | 0.12 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 18 | 0.12 |
| (1,1137) | 1:56:A:TYR:HA | 1:56:A:TYR:HD1 | 12 | 0.12 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 3 | 0.12 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 5 | 0.12 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 8 | 0.12 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 10 | 0.12 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 11 | 0.12 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 2 | 0.12 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 3 | 0.12 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 19 | 0.12 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 7 | 0.12 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 10 | 0.12 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 18 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 1 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 3 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 4 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 7 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|----------------|----------|---------------|
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 8 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 9 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 12 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 13 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 15 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 17 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 18 | 0.12 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 19 | 0.12 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 2 | 0.12 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 8 | 0.12 |
| (1,755) | 1:34:A:THR:HB | 1:35:A:LEU:H | 14 | 0.12 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 1 | 0.12 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 4 | 0.12 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 6 | 0.12 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 19 | 0.12 |
| (1,724) | 1:32:A:PHE:HA | 1:36:A:PHE:H | 10 | 0.12 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 2 | 0.12 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 2 | 0.12 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 5 | 0.12 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 13 | 0.12 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 15 | 0.12 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 20 | 0.12 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 18 | 0.12 |
| (1,552) | 1:22:A:ARG:HD2 | 1:32:A:PHE:HD2 | 5 | 0.12 |
| (1,552) | 1:22:A:ARG:HD2 | 1:32:A:PHE:HD2 | 6 | 0.12 |
| (1,402) | 1:18:A:LYS:HG3 | 1:19:A:TYR:H | 11 | 0.12 |
| (1,402) | 1:18:A:LYS:HG3 | 1:19:A:TYR:H | 14 | 0.12 |
| (1,395) | 1:18:A:LYS:HG2 | 1:18:A:LYS:H | 20 | 0.12 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 8 | 0.12 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 16 | 0.12 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 8 | 0.12 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 18 | 0.12 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 20 | 0.12 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 1 | 0.12 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 7 | 0.12 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 14 | 0.12 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 18 | 0.12 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 6 | 0.12 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 6 | 0.12 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 6 | 0.12 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 15 | 0.12 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 15 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|----------------|----------|---------------|
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 15 | 0.12 |
| (1,299) | 1:14:A:LEU:HD21 | 1:14:A:LEU:H | 18 | 0.12 |
| (1,299) | 1:14:A:LEU:HD22 | 1:14:A:LEU:H | 18 | 0.12 |
| (1,299) | 1:14:A:LEU:HD23 | 1:14:A:LEU:H | 18 | 0.12 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 4 | 0.12 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 4 | 0.12 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 6 | 0.12 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 8 | 0.12 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 11 | 0.12 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 14 | 0.12 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 17 | 0.12 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 1 | 0.12 |
| (1,178) | 1:8:A:HIS:HB2 | 1:9:A:HIS:HA | 7 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 1 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 3 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 4 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 8 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 16 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 18 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 19 | 0.12 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 20 | 0.12 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 2 | 0.12 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 4 | 0.12 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 5 | 0.12 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 14 | 0.12 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 15 | 0.12 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 5 | 0.12 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 8 | 0.12 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 11 | 0.12 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 16 | 0.12 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 18 | 0.12 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 20 | 0.12 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 10 | 0.12 |
| (1,9) | 1:2:A:THR:HB | 1:3:A:GLU:H | 10 | 0.12 |
| (1,8) | 1:2:A:THR:HG21 | 1:3:A:GLU:H | 11 | 0.12 |
| (1,8) | 1:2:A:THR:HG22 | 1:3:A:GLU:H | 11 | 0.12 |
| (1,8) | 1:2:A:THR:HG23 | 1:3:A:GLU:H | 11 | 0.12 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 1 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 3 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 5 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 10 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 15 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 16 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 17 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 19 | 0.11 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 20 | 0.11 |
| (1,1809) | 1:89:A:CYS:HA | 1:91:A:ASP:H | 11 | 0.11 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 2 | 0.11 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 3 | 0.11 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 8 | 0.11 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 10 | 0.11 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 11 | 0.11 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 3 | 0.11 |
| (1,1737) | 1:86:A:GLN:HG3 | 1:86:A:GLN:H | 10 | 0.11 |
| (1,1630) | 1:80:A:PHE:HB3 | 1:90:A:THR:H | 10 | 0.11 |
| (1,1630) | 1:80:A:PHE:HB3 | 1:90:A:THR:H | 19 | 0.11 |
| (1,1624) | 1:80:A:PHE:HD1 | 1:87:A:LEU:HG | 2 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 1 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 2 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 3 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 7 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 10 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 11 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 14 | 0.11 |
| (1,1623) | 1:80:A:PHE:HB2 | 1:87:A:LEU:HG | 20 | 0.11 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 1 | 0.11 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 7 | 0.11 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 10 | 0.11 |
| (1,1483) | 1:72:A:ARG:HB3 | 1:72:A:ARG:H | 13 | 0.11 |
| (1,1460) | 1:70:A:GLN:HG3 | 1:88:A:LEU:HG | 3 | 0.11 |
| (1,1407) | 1:68:A:CYS:HB2 | 1:89:A:CYS:HA | 19 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 1 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 4 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 7 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 9 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 11 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 12 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 13 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 15 | 0.11 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 20 | 0.11 |
| (1,1273) | 1:63:A:GLU:HA | 1:65:A:CYS:H | 10 | 0.11 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 3 | 0.11 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 7 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 12 | 0.11 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 17 | 0.11 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 7 | 0.11 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 14 | 0.11 |
| (1,1153) | 1:56:A:TYR:HB2 | 1:61:A:TRP:HZ3 | 8 | 0.11 |
| (1,1137) | 1:56:A:TYR:HA | 1:56:A:TYR:HD1 | 10 | 0.11 |
| (1,1137) | 1:56:A:TYR:HA | 1:56:A:TYR:HD1 | 18 | 0.11 |
| (1,1032) | 1:49:A:CYS:HA | 1:53:A:ASP:H | 19 | 0.11 |
| (1,953) | 1:42:A:GLU:HB2 | 1:65:A:CYS:HA | 9 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 1 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 4 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 5 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 7 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 10 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 11 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 14 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 15 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 17 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 18 | 0.11 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 20 | 0.11 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 1 | 0.11 |
| (1,897) | 1:40:A:CYS:HA | 1:61:A:TRP:HD1 | 15 | 0.11 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 2 | 0.11 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 5 | 0.11 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 6 | 0.11 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 10 | 0.11 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 11 | 0.11 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 14 | 0.11 |
| (1,857) | 1:39:A:THR:HB | 1:41:A:GLU:HG3 | 16 | 0.11 |
| (1,826) | 1:38:A:ASN:HB3 | 1:38:A:ASN:H | 18 | 0.11 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 3 | 0.11 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 17 | 0.11 |
| (1,724) | 1:32:A:PHE:HA | 1:36:A:PHE:H | 17 | 0.11 |
| (1,719) | 1:32:A:PHE:HA | 1:35:A:LEU:HG | 19 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 1 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 3 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 4 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 5 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 6 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 7 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 12 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|-----------------|----------|---------------|
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 15 | 0.11 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 20 | 0.11 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 1 | 0.11 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 3 | 0.11 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 9 | 0.11 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 12 | 0.11 |
| (1,677) | 1:30:A:VAL:HA | 1:33:A:GLU:H | 2 | 0.11 |
| (1,677) | 1:30:A:VAL:HA | 1:33:A:GLU:H | 4 | 0.11 |
| (1,655) | 1:29:A:VAL:HA | 1:32:A:PHE:HB2 | 2 | 0.11 |
| (1,655) | 1:29:A:VAL:HA | 1:32:A:PHE:HB2 | 4 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 8 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 11 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 12 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 13 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 15 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 16 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 19 | 0.11 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 20 | 0.11 |
| (1,518) | 1:22:A:ARG:HA | 1:22:A:ARG:HG3 | 3 | 0.11 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 12 | 0.11 |
| (1,415) | 1:19:A:TYR:HA | 1:20:A:ILE:HG12 | 1 | 0.11 |
| (1,415) | 1:19:A:TYR:HA | 1:20:A:ILE:HG12 | 3 | 0.11 |
| (1,415) | 1:19:A:TYR:HA | 1:20:A:ILE:HG12 | 7 | 0.11 |
| (1,402) | 1:18:A:LYS:HG3 | 1:19:A:TYR:H | 15 | 0.11 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 9 | 0.11 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 10 | 0.11 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 11 | 0.11 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 12 | 0.11 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 13 | 0.11 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 15 | 0.11 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 17 | 0.11 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 3 | 0.11 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 8 | 0.11 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 12 | 0.11 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 13 | 0.11 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 15 | 0.11 |
| (1,258) | 1:11:A:ASN:HB3 | 1:11:A:ASN:H | 19 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 1 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 3 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 7 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 12 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|----------------|----------|---------------|
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 16 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 18 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 19 | 0.11 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 20 | 0.11 |
| (1,162) | 1:7:A:CYS:HB3 | 1:28:A:CYS:H | 7 | 0.11 |
| (1,160) | 1:7:A:CYS:HB3 | 1:27:A:TYR:HA | 6 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 1 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 6 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 9 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 10 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 11 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 13 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 17 | 0.11 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 20 | 0.11 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 1 | 0.11 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 3 | 0.11 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 7 | 0.11 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 12 | 0.11 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 5 | 0.11 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 6 | 0.11 |
| (1,58) | 1:5:A:PHE:HB2 | 1:5:A:PHE:HD2 | 7 | 0.11 |
| (1,51) | 1:4:A:ARG:HB3 | 1:6:A:ASP:H | 11 | 0.11 |
| (1,51) | 1:4:A:ARG:HB3 | 1:6:A:ASP:H | 15 | 0.11 |
| (1,20) | 1:3:A:GLU:HB3 | 1:4:A:ARG:H | 5 | 0.11 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 2 | 0.11 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 4 | 0.11 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 8 | 0.11 |
| (1,9) | 1:2:A:THR:HB | 1:3:A:GLU:H | 6 | 0.11 |
| (1,8) | 1:2:A:THR:HG21 | 1:3:A:GLU:H | 12 | 0.11 |
| (1,8) | 1:2:A:THR:HG22 | 1:3:A:GLU:H | 12 | 0.11 |
| (1,8) | 1:2:A:THR:HG23 | 1:3:A:GLU:H | 12 | 0.11 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG2 | 17 | 0.1 |
| (1,1870) | 1:93:A:TYR:HE2 | 1:96:A:GLU:HG3 | 17 | 0.1 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 4 | 0.1 |
| (1,1860) | 1:93:A:TYR:HB2 | 1:94:A:SER:H | 12 | 0.1 |
| (1,1746) | 1:86:A:GLN:HG3 | 1:87:A:LEU:H | 15 | 0.1 |
| (1,1630) | 1:80:A:PHE:HB3 | 1:90:A:THR:H | 14 | 0.1 |
| (1,1630) | 1:80:A:PHE:HB3 | 1:90:A:THR:H | 16 | 0.1 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 5 | 0.1 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 9 | 0.1 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 14 | 0.1 |
| (1,1526) | 1:75:A:LEU:HA | 1:78:A:LYS:HB3 | 16 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 2 | 0.1 |
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 4 | 0.1 |
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 5 | 0.1 |
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 12 | 0.1 |
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 15 | 0.1 |
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 18 | 0.1 |
| (1,1494) | 1:73:A:ASN:HB2 | 1:73:A:ASN:HD22 | 20 | 0.1 |
| (1,1460) | 1:70:A:GLN:HG3 | 1:88:A:LEU:HG | 10 | 0.1 |
| (1,1460) | 1:70:A:GLN:HG3 | 1:88:A:LEU:HG | 14 | 0.1 |
| (1,1407) | 1:68:A:CYS:HB2 | 1:89:A:CYS:HA | 1 | 0.1 |
| (1,1407) | 1:68:A:CYS:HB2 | 1:89:A:CYS:HA | 9 | 0.1 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 5 | 0.1 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 6 | 0.1 |
| (1,1401) | 1:68:A:CYS:HA | 1:87:A:LEU:HB2 | 17 | 0.1 |
| (1,1381) | 1:68:A:CYS:HB2 | 1:72:A:ARG:HA | 17 | 0.1 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD21 | 4 | 0.1 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD22 | 4 | 0.1 |
| (1,1339) | 1:66:A:PHE:HD2 | 1:87:A:LEU:HD23 | 4 | 0.1 |
| (1,1273) | 1:63:A:GLU:HA | 1:65:A:CYS:H | 3 | 0.1 |
| (1,1273) | 1:63:A:GLU:HA | 1:65:A:CYS:H | 7 | 0.1 |
| (1,1192) | 1:59:A:ARG:HG2 | 1:59:A:ARG:H | 4 | 0.1 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 3 | 0.1 |
| (1,1167) | 1:57:A:LYS:HB3 | 1:57:A:LYS:H | 12 | 0.1 |
| (1,1153) | 1:56:A:TYR:HB2 | 1:61:A:TRP:HZ3 | 13 | 0.1 |
| (1,1137) | 1:56:A:TYR:HA | 1:56:A:TYR:HD1 | 7 | 0.1 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 6 | 0.1 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 8 | 0.1 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 12 | 0.1 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 13 | 0.1 |
| (1,914) | 1:41:A:GLU:HB3 | 1:42:A:GLU:H | 16 | 0.1 |
| (1,874) | 1:40:A:CYS:HA | 1:41:A:GLU:HG3 | 10 | 0.1 |
| (1,826) | 1:38:A:ASN:HB3 | 1:38:A:ASN:H | 5 | 0.1 |
| (1,729) | 1:33:A:GLU:HB3 | 1:33:A:GLU:H | 5 | 0.1 |
| (1,724) | 1:32:A:PHE:HA | 1:36:A:PHE:H | 12 | 0.1 |
| (1,719) | 1:32:A:PHE:HA | 1:35:A:LEU:HG | 2 | 0.1 |
| (1,719) | 1:32:A:PHE:HA | 1:35:A:LEU:HG | 17 | 0.1 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 9 | 0.1 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 10 | 0.1 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 11 | 0.1 |
| (1,701) | 1:31:A:CYS:HB3 | 1:35:A:LEU:H | 14 | 0.1 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 6 | 0.1 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 7 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|----------------|----------|---------------|
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 8 | 0.1 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 14 | 0.1 |
| (1,699) | 1:31:A:CYS:HB3 | 1:35:A:LEU:HG | 18 | 0.1 |
| (1,677) | 1:30:A:VAL:HA | 1:33:A:GLU:H | 6 | 0.1 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 9 | 0.1 |
| (1,610) | 1:27:A:TYR:HA | 1:28:A:CYS:HB3 | 10 | 0.1 |
| (1,541) | 1:22:A:ARG:HG3 | 1:27:A:TYR:HD1 | 6 | 0.1 |
| (1,506) | 1:21:A:LEU:HB3 | 1:25:A:SER:HA | 11 | 0.1 |
| (1,499) | 1:21:A:LEU:HB3 | 1:22:A:ARG:H | 20 | 0.1 |
| (1,391) | 1:18:A:LYS:HA | 1:18:A:LYS:HG2 | 5 | 0.1 |
| (1,316) | 1:14:A:LEU:HG | 1:19:A:TYR:HD2 | 3 | 0.1 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 9 | 0.1 |
| (1,312) | 1:14:A:LEU:HB2 | 1:17:A:LYS:H | 17 | 0.1 |
| (1,202) | 1:8:A:HIS:H | 1:27:A:TYR:HA | 15 | 0.1 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 7 | 0.1 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 8 | 0.1 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 16 | 0.1 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 18 | 0.1 |
| (1,143) | 1:7:A:CYS:HA | 1:14:A:LEU:H | 19 | 0.1 |
| (1,136) | 1:7:A:CYS:HB3 | 1:12:A:GLU:HG3 | 13 | 0.1 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 2 | 0.1 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 7 | 0.1 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 10 | 0.1 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 14 | 0.1 |
| (1,73) | 1:5:A:PHE:HZ | 1:14:A:LEU:HB3 | 18 | 0.1 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 13 | 0.1 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 14 | 0.1 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 15 | 0.1 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 19 | 0.1 |
| (1,14) | 1:3:A:GLU:HB2 | 1:3:A:GLU:H | 20 | 0.1 |

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

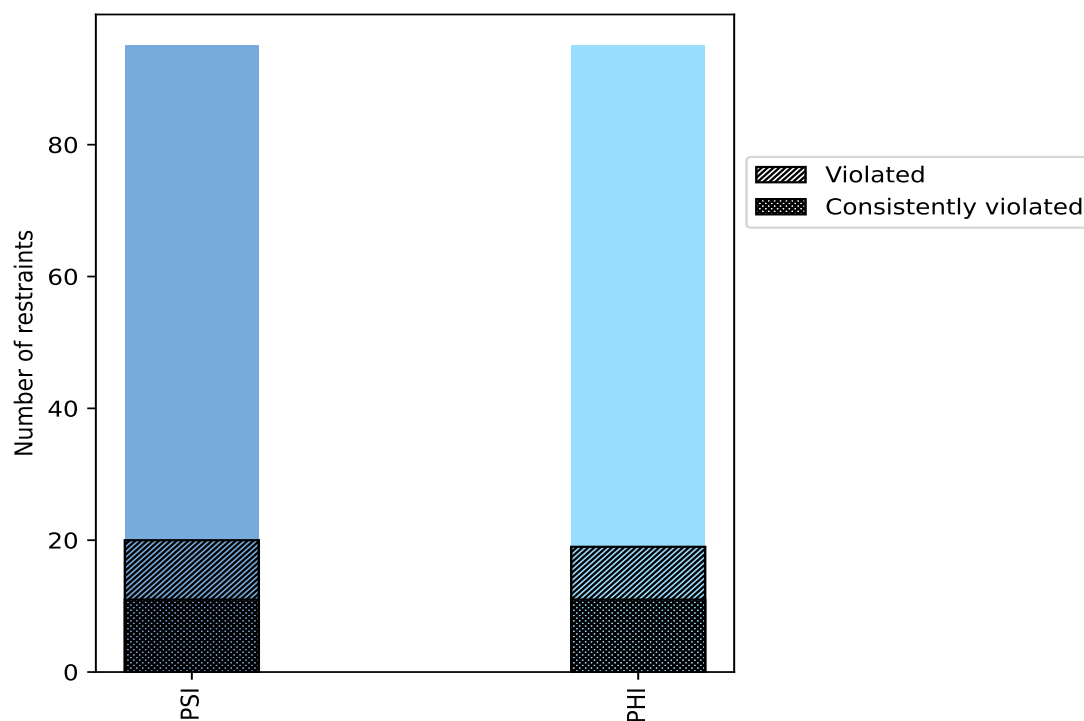
10.1 Summary of dihedral-angle violations [i](#)

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 | 95 | 50.0 | 20 | 21.1 | 10.5 | 11 | 11.6 | 5.8 |
| PHI | 95 | 50.0 | 19 | 20.0 | 10.0 | 11 | 11.6 | 5.8 |
| Total | 190 | 100.0 | 39 | 20.5 | 20.5 | 22 | 11.6 | 11.6 |

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](#)



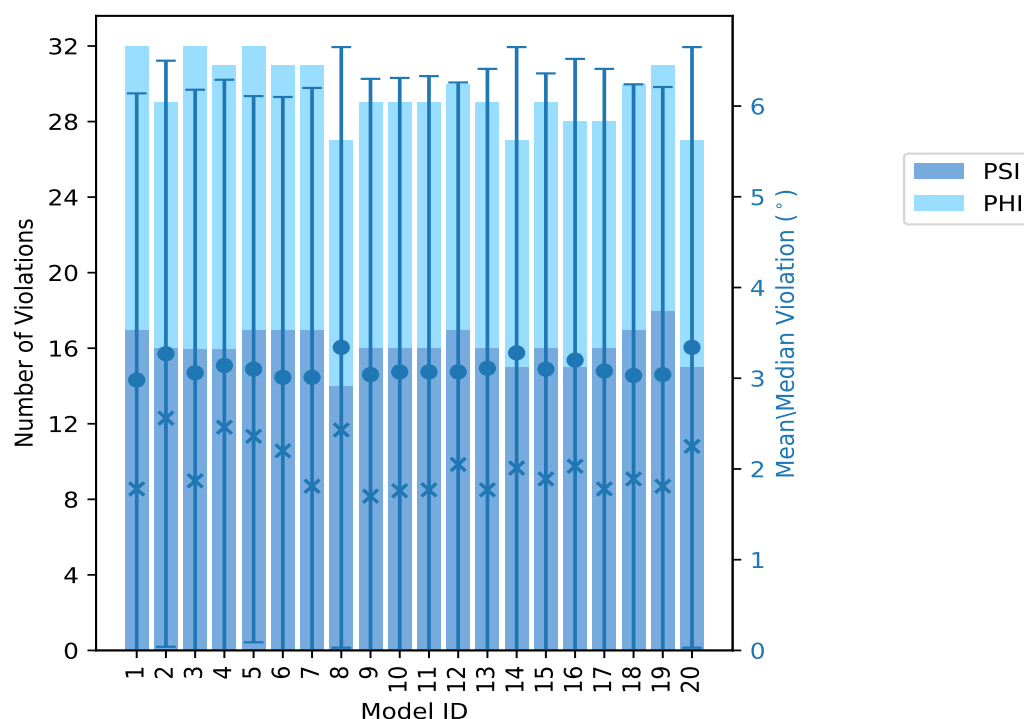
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 | 17 | 15 | 32 | 2.98 | 15.43 | 3.16 | 1.78 |
| 2 | 16 | 13 | 29 | 3.27 | 15.1 | 3.23 | 2.56 |
| 3 | 16 | 16 | 32 | 3.06 | 15.11 | 3.12 | 1.87 |
| 4 | 16 | 15 | 31 | 3.14 | 15.37 | 3.15 | 2.46 |
| 5 | 17 | 15 | 32 | 3.1 | 14.59 | 3.01 | 2.36 |
| 6 | 17 | 14 | 31 | 3.01 | 14.79 | 3.09 | 2.2 |
| 7 | 17 | 14 | 31 | 3.01 | 15.21 | 3.19 | 1.81 |
| 8 | 14 | 13 | 27 | 3.34 | 15.33 | 3.31 | 2.43 |
| 9 | 16 | 13 | 29 | 3.04 | 15.11 | 3.26 | 1.7 |
| 10 | 16 | 13 | 29 | 3.07 | 15.1 | 3.24 | 1.76 |
| 11 | 16 | 13 | 29 | 3.07 | 15.27 | 3.26 | 1.77 |
| 12 | 17 | 13 | 30 | 3.07 | 15.19 | 3.19 | 2.05 |
| 13 | 16 | 13 | 29 | 3.11 | 15.57 | 3.3 | 1.77 |
| 14 | 15 | 12 | 27 | 3.28 | 15.41 | 3.37 | 2.01 |
| 15 | 16 | 13 | 29 | 3.1 | 15.2 | 3.26 | 1.89 |
| 16 | 15 | 13 | 28 | 3.2 | 15.27 | 3.32 | 2.03 |
| 17 | 16 | 12 | 28 | 3.08 | 15.34 | 3.33 | 1.78 |
| 18 | 17 | 13 | 30 | 3.03 | 15.21 | 3.21 | 1.89 |
| 19 | 18 | 13 | 31 | 3.04 | 15.18 | 3.17 | 1.81 |
| 20 | 15 | 12 | 27 | 3.34 | 15.31 | 3.31 | 2.25 |

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



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

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

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

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

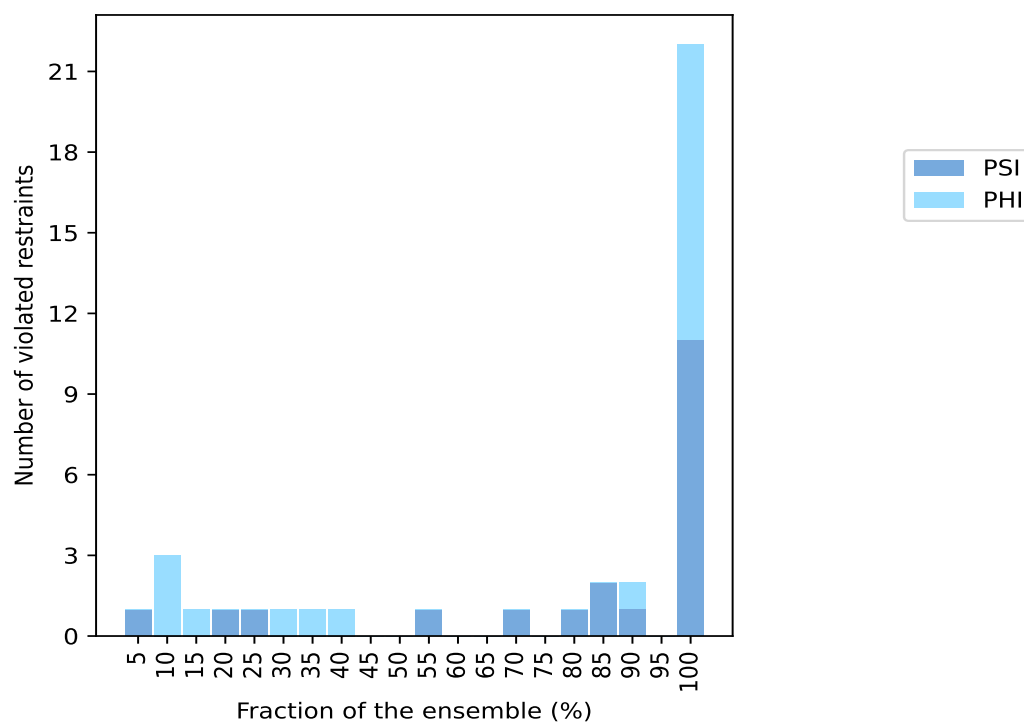
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 0 | 0 | 0 | 13 | 65.0 |
| 1 | 0 | 1 | 14 | 70.0 |
| 0 | 0 | 0 | 15 | 75.0 |
| 1 | 0 | 1 | 16 | 80.0 |
| 2 | 0 | 2 | 17 | 85.0 |
| 1 | 1 | 2 | 18 | 90.0 |
| 0 | 0 | 0 | 19 | 95.0 |
| 11 | 11 | 22 | 20 | 100.0 |

¹ Number of models with violations

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

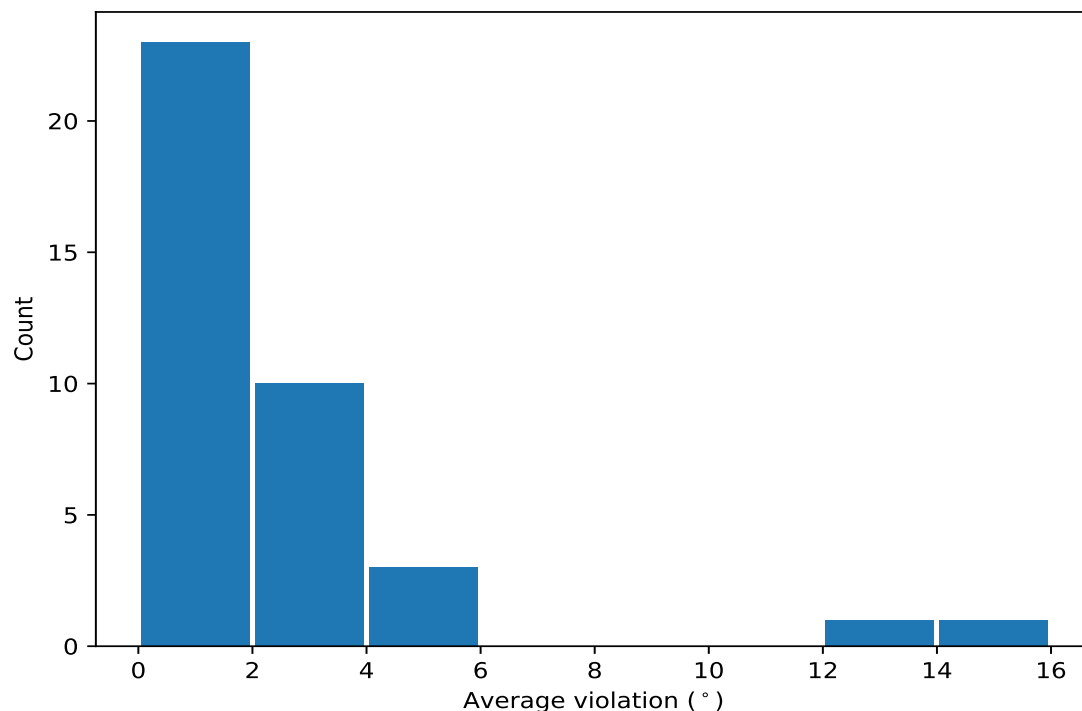


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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 |
|---------|--------------|---------------|---------------|--------------|---------------------|-------|-----------------|--------|
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 20 | 15.2 | 0.21 | 15.21 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 20 | 13.31 | 0.13 | 13.34 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 20 | 5.21 | 0.22 | 5.18 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 20 | 5.1 | 0.23 | 5.04 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 20 | 4.08 | 0.14 | 4.06 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 20 | 3.99 | 0.37 | 4.07 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 20 | 3.63 | 0.21 | 3.67 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 20 | 2.85 | 0.52 | 2.82 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 20 | 2.83 | 0.15 | 2.8 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 20 | 2.64 | 0.18 | 2.6 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 20 | 2.6 | 0.22 | 2.6 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 20 | 2.49 | 0.21 | 2.49 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 20 | 2.34 | 0.57 | 2.45 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 20 | 2.11 | 0.48 | 2.3 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 20 | 1.96 | 0.37 | 1.9 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 20 | 1.86 | 0.52 | 1.82 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 20 | 1.72 | 0.15 | 1.74 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 20 | 1.72 | 0.2 | 1.71 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 20 | 1.53 | 0.16 | 1.5 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 20 | 1.48 | 0.17 | 1.46 |

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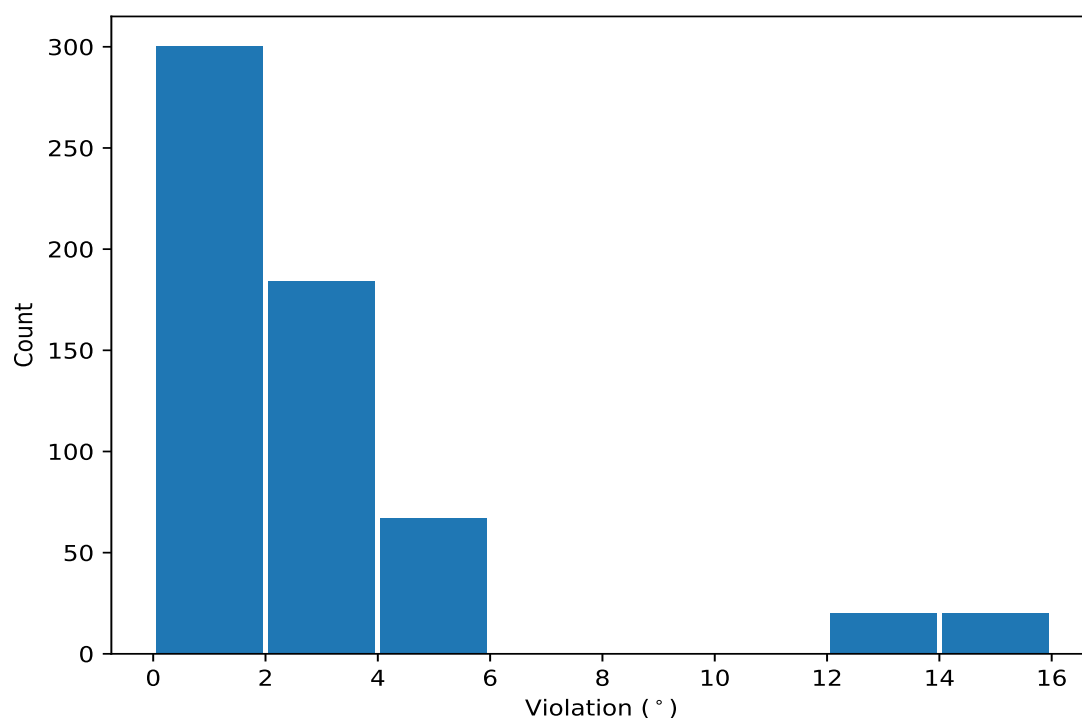
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|--------------|---------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 20 | 1.45 | 0.15 | 1.4 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 20 | 1.35 | 0.16 | 1.3 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 18 | 1.55 | 0.36 | 1.54 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 18 | 1.48 | 0.27 | 1.48 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 17 | 1.4 | 0.26 | 1.42 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 17 | 1.16 | 0.1 | 1.13 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 16 | 1.21 | 0.13 | 1.18 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 14 | 1.45 | 0.56 | 1.23 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 11 | 1.31 | 0.17 | 1.25 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 8 | 1.09 | 0.04 | 1.1 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 7 | 2.72 | 0.9 | 3.15 |
| (1,131) | 1:66:A:PHE:C | 1:67:A:HIS:N | 1:67:A:HIS:CA | 1:67:A:HIS:C | 6 | 1.12 | 0.09 | 1.07 |
| (1,116) | 1:59:A:ARG:N | 1:59:A:ARG:CA | 1:59:A:ARG:C | 1:60:A:HIS:N | 5 | 1.08 | 0.05 | 1.1 |
| (1,190) | 1:96:A:GLU:N | 1:96:A:GLU:CA | 1:96:A:GLU:C | 1:97:A:TYR:N | 4 | 1.5 | 0.25 | 1.49 |
| (1,57) | 1:29:A:VAL:C | 1:30:A:VAL:N | 1:30:A:VAL:CA | 1:30:A:VAL:C | 3 | 1.46 | 0.18 | 1.46 |
| (1,33) | 1:17:A:LYS:C | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 2 | 1.42 | 0.18 | 1.42 |
| (1,19) | 1:10:A:CYS:C | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 2 | 1.34 | 0.04 | 1.34 |
| (1,47) | 1:24:A:GLU:C | 1:25:A:SER:N | 1:25:A:SER:CA | 1:25:A:SER:C | 2 | 1.02 | 0.01 | 1.02 |

¹ Number of violated models, ²Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|--------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 13 | 15.57 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 1 | 15.43 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 14 | 15.41 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 4 | 15.37 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 17 | 15.34 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 8 | 15.33 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 20 | 15.31 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 11 | 15.27 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 16 | 15.27 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 7 | 15.21 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 18 | 15.21 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 15 | 15.2 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 12 | 15.19 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 19 | 15.18 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 3 | 15.11 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 9 | 15.11 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 2 | 15.1 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 10 | 15.1 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 6 | 14.79 |
| (1,29) | 1:15:A:PHE:C | 1:16:A:GLY:N | 1:16:A:GLY:CA | 1:16:A:GLY:C | 5 | 14.59 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 2 | 13.44 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 1 | 13.43 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 3 | 13.43 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 4 | 13.41 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 9 | 13.4 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 16 | 13.4 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 7 | 13.39 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 14 | 13.39 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 20 | 13.38 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 17 | 13.35 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 8 | 13.34 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 10 | 13.31 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 12 | 13.31 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 15 | 13.29 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 18 | 13.29 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 19 | 13.21 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 11 | 13.2 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 13 | 13.17 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 5 | 13.11 |
| (1,28) | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1:16:A:GLY:N | 6 | 12.91 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 6 | 5.72 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 7 | 5.6 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 2 | 5.44 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 5 | 5.42 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 19 | 5.41 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 5 | 5.41 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 17 | 5.39 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 16 | 5.36 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 11 | 5.36 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 13 | 5.35 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 14 | 5.33 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 3 | 5.32 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 18 | 5.32 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 1 | 5.3 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 4 | 5.21 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 20 | 5.2 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 2 | 5.19 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 15 | 5.18 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 9 | 5.14 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 12 | 5.12 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 8 | 5.1 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 10 | 5.1 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 1 | 5.07 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 13 | 5.06 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 4 | 5.05 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 15 | 5.04 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 8 | 5.03 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 19 | 5.03 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 9 | 5.02 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 16 | 5.02 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 6 | 5.01 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 10 | 5.0 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 14 | 5.0 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 12 | 4.93 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 7 | 4.92 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 3 | 4.9 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 18 | 4.9 |
| (1,27) | 1:14:A:LEU:C | 1:15:A:PHE:N | 1:15:A:PHE:CA | 1:15:A:PHE:C | 20 | 4.83 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 17 | 4.78 |
| (1,148) | 1:75:A:LEU:N | 1:75:A:LEU:CA | 1:75:A:LEU:C | 1:76:A:VAL:N | 11 | 4.58 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 20 | 4.49 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 3 | 4.47 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 13 | 4.46 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 14 | 4.45 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 19 | 4.34 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 16 | 4.3 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 15 | 4.29 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 6 | 4.26 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 7 | 4.25 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 14 | 4.23 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 5 | 4.21 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 2 | 4.2 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 8 | 4.19 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 12 | 4.17 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 19 | 4.16 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 5 | 4.16 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 13 | 4.15 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 3 | 4.14 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 8 | 4.11 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 18 | 4.1 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 16 | 4.09 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 4 | 4.06 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 18 | 4.05 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 16 | 4.05 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 1 | 4.01 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 2 | 4.01 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 17 | 4.01 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 11 | 3.99 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 10 | 3.98 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 3 | 3.96 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 15 | 3.96 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 12 | 3.95 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 9 | 3.95 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 6 | 3.92 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 15 | 3.92 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 20 | 3.88 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 10 | 3.86 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 8 | 3.85 |
| (1,165) | 1:83:A:LYS:C | 1:84:A:GLU:N | 1:84:A:GLU:CA | 1:84:A:GLU:C | 9 | 3.83 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 9 | 3.79 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 17 | 3.79 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 14 | 3.75 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 3 | 3.73 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 7 | 3.72 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 11 | 3.72 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 10 | 3.71 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 11 | 3.71 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 13 | 3.7 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 4 | 3.7 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 2 | 3.68 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 11 | 3.67 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 5 | 3.64 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 1 | 3.63 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 19 | 3.54 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 18 | 3.52 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 7 | 3.5 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 12 | 3.48 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 2 | 3.46 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 6 | 3.42 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 15 | 3.4 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 5 | 3.39 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 4 | 3.36 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 17 | 3.35 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 20 | 3.33 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 4 | 3.22 |
| (1,164) | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1:84:A:GLU:N | 20 | 3.19 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 6 | 3.15 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 18 | 3.14 |
| (1,149) | 1:75:A:LEU:C | 1:76:A:VAL:N | 1:76:A:VAL:CA | 1:76:A:VAL:C | 1 | 3.13 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 8 | 3.1 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 1 | 3.1 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 20 | 3.09 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 4 | 3.07 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 7 | 3.05 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 11 | 3.01 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 10 | 3.0 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 1 | 2.99 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 2 | 2.99 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 7 | 2.96 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 10 | 2.95 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 19 | 2.95 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 4 | 2.93 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 9 | 2.93 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 19 | 2.92 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 2 | 2.91 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 2 | 2.9 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 7 | 2.89 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 16 | 2.89 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 19 | 2.88 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 2 | 2.88 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 12 | 2.86 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 19 | 2.85 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 2 | 2.84 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 12 | 2.83 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 13 | 2.82 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 5 | 2.82 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 14 | 2.81 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 5 | 2.81 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 3 | 2.8 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 10 | 2.8 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 15 | 2.8 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 19 | 2.8 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 14 | 2.8 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 9 | 2.79 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 17 | 2.78 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 1 | 2.78 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 3 | 2.78 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 5 | 2.78 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 18 | 2.77 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 6 | 2.77 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 3 | 2.76 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 17 | 2.76 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 20 | 2.76 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 6 | 2.75 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 16 | 2.75 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 16 | 2.74 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 17 | 2.74 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 13 | 2.73 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 16 | 2.72 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 16 | 2.72 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 4 | 2.71 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 18 | 2.71 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 14 | 2.7 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 5 | 2.7 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 6 | 2.68 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 2 | 2.65 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 11 | 2.65 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 4 | 2.64 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 17 | 2.64 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 8 | 2.64 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 8 | 2.64 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 13 | 2.64 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 4 | 2.63 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 9 | 2.62 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 8 | 2.62 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 5 | 2.61 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 20 | 2.6 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 20 | 2.6 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 10 | 2.58 |
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 20 | 2.58 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 7 | 2.57 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 19 | 2.57 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 12 | 2.57 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 10 | 2.57 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 12 | 2.56 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,161) | 1:81:A:ALA:C | 1:82:A:ALA:N | 1:82:A:ALA:CA | 1:82:A:ALA:C | 2 | 2.56 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 19 | 2.55 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 1 | 2.55 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 5 | 2.55 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 13 | 2.55 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 8 | 2.54 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 14 | 2.54 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 11 | 2.53 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 1 | 2.53 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 15 | 2.5 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 4 | 2.49 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 14 | 2.49 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 4 | 2.48 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 13 | 2.48 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 15 | 2.48 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 12 | 2.48 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 9 | 2.47 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 6 | 2.47 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 13 | 2.47 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 11 | 2.47 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 16 | 2.47 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 4 | 2.46 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 8 | 2.46 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 18 | 2.44 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 15 | 2.44 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 8 | 2.43 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 14 | 2.43 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 12 | 2.43 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 5 | 2.41 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 5 | 2.4 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 7 | 2.4 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 6 | 2.39 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 6 | 2.38 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 9 | 2.38 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 11 | 2.35 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 1 | 2.34 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 16 | 2.34 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 3 | 2.34 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 1 | 2.33 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 18 | 2.33 |
| (1,170) | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1:87:A:LEU:N | 5 | 2.32 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 8 | 2.3 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 7 | 2.3 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 12 | 2.28 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 2 | 2.27 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 12 | 2.27 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 6 | 2.26 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 7 | 2.26 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 15 | 2.26 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 20 | 2.25 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 1 | 2.24 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 17 | 2.21 |
| (1,175) | 1:88:A:LEU:C | 1:89:A:CYS:N | 1:89:A:CYS:CA | 1:89:A:CYS:C | 15 | 2.2 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 6 | 2.2 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 9 | 2.19 |
| (1,25) | 1:13:A:SER:C | 1:14:A:LEU:N | 1:14:A:LEU:CA | 1:14:A:LEU:C | 5 | 2.19 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 20 | 2.18 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 4 | 2.16 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 7 | 2.13 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 8 | 2.1 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 20 | 2.09 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 18 | 2.09 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 18 | 2.06 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 10 | 2.01 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 14 | 2.01 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 2 | 2.0 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 3 | 1.98 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 13 | 1.98 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 5 | 1.97 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 3 | 1.96 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 4 | 1.96 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 18 | 1.96 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 20 | 1.95 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 11 | 1.94 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 4 | 1.91 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 9 | 1.9 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 15 | 1.89 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 14 | 1.89 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 14 | 1.89 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 20 | 1.89 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 3 | 1.89 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 3 | 1.87 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 3 | 1.87 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 5 | 1.86 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 17 | 1.85 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 14 | 1.85 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 19 | 1.85 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 20 | 1.84 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 10 | 1.83 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 5 | 1.83 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 12 | 1.83 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 3 | 1.82 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 18 | 1.82 |
| (1,34) | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 1:19:A:TYR:N | 17 | 1.82 |
| (1,190) | 1:96:A:GLU:N | 1:96:A:GLU:CA | 1:96:A:GLU:C | 1:97:A:TYR:N | 3 | 1.81 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 8 | 1.81 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 6 | 1.81 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 19 | 1.81 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 7 | 1.81 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 19 | 1.8 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 6 | 1.8 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 1 | 1.8 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 7 | 1.79 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 12 | 1.78 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 19 | 1.78 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 11 | 1.77 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 13 | 1.77 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 3 | 1.77 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 12 | 1.77 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 1 | 1.77 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 15 | 1.76 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 10 | 1.76 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 2 | 1.75 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 18 | 1.74 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 17 | 1.74 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 12 | 1.73 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 8 | 1.73 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 1 | 1.73 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 13 | 1.72 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 16 | 1.72 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 19 | 1.72 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 10 | 1.72 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 2 | 1.71 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 17 | 1.71 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 9 | 1.7 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 4 | 1.7 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 7 | 1.7 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 18 | 1.7 |
| (1,190) | 1:96:A:GLU:N | 1:96:A:GLU:CA | 1:96:A:GLU:C | 1:97:A:TYR:N | 18 | 1.69 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 10 | 1.69 |
| (1,57) | 1:29:A:VAL:C | 1:30:A:VAL:N | 1:30:A:VAL:CA | 1:30:A:VAL:C | 3 | 1.69 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 1 | 1.68 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 14 | 1.68 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 9 | 1.67 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 8 | 1.67 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 11 | 1.66 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 13 | 1.66 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 1 | 1.66 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 3 | 1.65 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 15 | 1.65 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 10 | 1.65 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 18 | 1.64 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 9 | 1.64 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 13 | 1.64 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 19 | 1.64 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 16 | 1.63 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 11 | 1.63 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 9 | 1.63 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 8 | 1.63 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 3 | 1.63 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 15 | 1.63 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 3 | 1.63 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 1 | 1.62 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 9 | 1.62 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 3 | 1.62 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 6 | 1.62 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 7 | 1.62 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 16 | 1.62 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 6 | 1.61 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 8 | 1.6 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 8 | 1.6 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 4 | 1.6 |
| (1,33) | 1:17:A:LYS:C | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 5 | 1.6 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 17 | 1.59 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 13 | 1.58 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 19 | 1.58 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 9 | 1.58 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 16 | 1.58 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 17 | 1.57 |
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 20 | 1.56 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 15 | 1.56 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 10 | 1.56 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 12 | 1.56 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 14 | 1.56 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 9 | 1.55 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 4 | 1.55 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 8 | 1.54 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 3 | 1.54 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 5 | 1.53 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 11 | 1.53 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 7 | 1.53 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 11 | 1.53 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 10 | 1.52 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 11 | 1.52 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 16 | 1.52 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 18 | 1.52 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 7 | 1.51 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 17 | 1.51 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 12 | 1.5 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 11 | 1.5 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 10 | 1.49 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 1 | 1.49 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 5 | 1.49 |
| (1,114) | 1:58:A:ASP:N | 1:58:A:ASP:CA | 1:58:A:ASP:C | 1:59:A:ARG:N | 13 | 1.49 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 6 | 1.49 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 14 | 1.48 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 20 | 1.48 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 8 | 1.48 |
| (1,41) | 1:21:A:LEU:C | 1:22:A:ARG:N | 1:22:A:ARG:CA | 1:22:A:ARG:C | 7 | 1.48 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 12 | 1.48 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 11 | 1.47 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 12 | 1.47 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 6 | 1.47 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 16 | 1.46 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 12 | 1.46 |
| (1,57) | 1:29:A:VAL:C | 1:30:A:VAL:N | 1:30:A:VAL:CA | 1:30:A:VAL:C | 1 | 1.46 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 3 | 1.45 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 17 | 1.45 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 7 | 1.45 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 4 | 1.45 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 2 | 1.45 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 10 | 1.45 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 20 | 1.44 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 4 | 1.44 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 6 | 1.43 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 15 | 1.43 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 1 | 1.43 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 15 | 1.42 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 17 | 1.42 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 19 | 1.41 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 2 | 1.41 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 9 | 1.41 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 13 | 1.41 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 10 | 1.4 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 12 | 1.4 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 7 | 1.4 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 1 | 1.39 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 20 | 1.39 |
| (1,19) | 1:10:A:CYS:C | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 15 | 1.39 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 20 | 1.38 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 9 | 1.38 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 15 | 1.38 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 16 | 1.36 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 1 | 1.36 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1 | 1.36 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 14 | 1.36 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 17 | 1.36 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 2 | 1.36 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 4 | 1.36 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 2 | 1.36 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 13 | 1.35 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 16 | 1.35 |
| (1,60) | 1:31:A:CYS:N | 1:31:A:CYS:CA | 1:31:A:CYS:C | 1:32:A:PHE:N | 16 | 1.35 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 18 | 1.34 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 18 | 1.34 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 14 | 1.33 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 10 | 1.33 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 3 | 1.33 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 11 | 1.32 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 14 | 1.32 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 18 | 1.32 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 4 | 1.32 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 16 | 1.32 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 20 | 1.32 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 11 | 1.32 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,138) | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 1:71:A:CYS:N | 18 | 1.31 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 1 | 1.31 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 2 | 1.3 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 5 | 1.3 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 6 | 1.3 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 19 | 1.3 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 13 | 1.3 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 16 | 1.3 |
| (1,19) | 1:10:A:CYS:C | 1:11:A:ASN:N | 1:11:A:ASN:CA | 1:11:A:ASN:C | 13 | 1.3 |
| (1,190) | 1:96:A:GLU:N | 1:96:A:GLU:CA | 1:96:A:GLU:C | 1:97:A:TYR:N | 12 | 1.29 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 4 | 1.29 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 7 | 1.29 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 10 | 1.29 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 17 | 1.29 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 5 | 1.29 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 17 | 1.28 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 17 | 1.27 |
| (1,154) | 1:78:A:LYS:N | 1:78:A:LYS:CA | 1:78:A:LYS:C | 1:79:A:PRO:N | 14 | 1.27 |
| (1,131) | 1:66:A:PHE:C | 1:67:A:HIS:N | 1:67:A:HIS:CA | 1:67:A:HIS:C | 4 | 1.27 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 2 | 1.27 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 10 | 1.26 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 14 | 1.25 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 13 | 1.25 |
| (1,33) | 1:17:A:LYS:C | 1:18:A:LYS:N | 1:18:A:LYS:CA | 1:18:A:LYS:C | 3 | 1.25 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 6 | 1.24 |
| (1,57) | 1:29:A:VAL:C | 1:30:A:VAL:N | 1:30:A:VAL:CA | 1:30:A:VAL:C | 4 | 1.24 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 18 | 1.23 |
| (1,190) | 1:96:A:GLU:N | 1:96:A:GLU:CA | 1:96:A:GLU:C | 1:97:A:TYR:N | 5 | 1.22 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 13 | 1.22 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 14 | 1.22 |
| (1,163) | 1:82:A:ALA:C | 1:83:A:LYS:N | 1:83:A:LYS:CA | 1:83:A:LYS:C | 2 | 1.21 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 1 | 1.21 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 16 | 1.21 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 7 | 1.21 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 15 | 1.21 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 11 | 1.2 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 4 | 1.2 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 19 | 1.2 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 2 | 1.19 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 5 | 1.19 |
| (1,131) | 1:66:A:PHE:C | 1:67:A:HIS:N | 1:67:A:HIS:CA | 1:67:A:HIS:C | 6 | 1.19 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 19 | 1.18 |
| (1,137) | 1:69:A:SER:C | 1:70:A:GLN:N | 1:70:A:GLN:CA | 1:70:A:GLN:C | 7 | 1.18 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 9 | 1.18 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 19 | 1.18 |
| (1,68) | 1:35:A:LEU:N | 1:35:A:LEU:CA | 1:35:A:LEU:C | 1:36:A:PHE:N | 8 | 1.18 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 12 | 1.17 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 10 | 1.17 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 18 | 1.17 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 18 | 1.17 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 7 | 1.17 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 9 | 1.16 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 15 | 1.16 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 2 | 1.15 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 20 | 1.15 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 14 | 1.14 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 12 | 1.14 |
| (1,116) | 1:59:A:ARG:N | 1:59:A:ARG:CA | 1:59:A:ARG:C | 1:60:A:HIS:N | 19 | 1.14 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 4 | 1.14 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 19 | 1.14 |
| (1,169) | 1:85:A:ASP:C | 1:86:A:GLN:N | 1:86:A:GLN:CA | 1:86:A:GLN:C | 15 | 1.13 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 8 | 1.13 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 5 | 1.13 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 5 | 1.13 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 5 | 1.13 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 1 | 1.12 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 9 | 1.12 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 7 | 1.12 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 17 | 1.12 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 3 | 1.11 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 6 | 1.11 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 19 | 1.11 |
| (1,116) | 1:59:A:ARG:N | 1:59:A:ARG:CA | 1:59:A:ARG:C | 1:60:A:HIS:N | 2 | 1.11 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 18 | 1.1 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 3 | 1.1 |
| (1,116) | 1:59:A:ARG:N | 1:59:A:ARG:CA | 1:59:A:ARG:C | 1:60:A:HIS:N | 17 | 1.1 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 13 | 1.09 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 13 | 1.09 |
| (1,74) | 1:38:A:ASN:N | 1:38:A:ASN:CA | 1:38:A:ASN:C | 1:39:A:THR:N | 15 | 1.09 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 6 | 1.09 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 3 | 1.08 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 15 | 1.08 |
| (1,64) | 1:33:A:GLU:N | 1:33:A:GLU:CA | 1:33:A:GLU:C | 1:34:A:THR:N | 12 | 1.08 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 10 | 1.07 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 11 | 1.07 |
| (1,131) | 1:66:A:PHE:C | 1:67:A:HIS:N | 1:67:A:HIS:CA | 1:67:A:HIS:C | 1 | 1.07 |
| (1,131) | 1:66:A:PHE:C | 1:67:A:HIS:N | 1:67:A:HIS:CA | 1:67:A:HIS:C | 17 | 1.07 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 15 | 1.07 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 12 | 1.06 |
| (1,146) | 1:74:A:SER:N | 1:74:A:SER:CA | 1:74:A:SER:C | 1:75:A:LEU:N | 6 | 1.06 |
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 9 | 1.06 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 16 | 1.06 |
| (1,131) | 1:66:A:PHE:C | 1:67:A:HIS:N | 1:67:A:HIS:CA | 1:67:A:HIS:C | 19 | 1.06 |
| (1,125) | 1:63:A:GLU:C | 1:64:A:ALA:N | 1:64:A:ALA:CA | 1:64:A:ALA:C | 11 | 1.06 |
| (1,134) | 1:68:A:CYS:N | 1:68:A:CYS:CA | 1:68:A:CYS:C | 1:69:A:SER:N | 6 | 1.05 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 9 | 1.05 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 13 | 1.05 |
| (1,131) | 1:66:A:PHE:C | 1:67:A:HIS:N | 1:67:A:HIS:CA | 1:67:A:HIS:C | 11 | 1.03 |
| (1,116) | 1:59:A:ARG:N | 1:59:A:ARG:CA | 1:59:A:ARG:C | 1:60:A:HIS:N | 9 | 1.03 |
| (1,84) | 1:43:A:CYS:N | 1:43:A:CYS:CA | 1:43:A:CYS:C | 1:44:A:GLY:N | 19 | 1.03 |
| (1,47) | 1:24:A:GLU:C | 1:25:A:SER:N | 1:25:A:SER:CA | 1:25:A:SER:C | 16 | 1.03 |
| (1,167) | 1:84:A:GLU:C | 1:85:A:ASP:N | 1:85:A:ASP:CA | 1:85:A:ASP:C | 7 | 1.02 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,142) | 1:72:A:ARG:N | 1:72:A:ARG:CA | 1:72:A:ARG:C | 1:73:A:ASN:N | 20 | 1.02 |
| (1,8) | 1:5:A:PHE:N | 1:5:A:PHE:CA | 1:5:A:PHE:C | 1:6:A:ASP:N | 8 | 1.02 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 7 | 1.01 |
| (1,129) | 1:65:A:CYS:C | 1:66:A:PHE:N | 1:66:A:PHE:CA | 1:66:A:PHE:C | 11 | 1.01 |
| (1,47) | 1:24:A:GLU:C | 1:25:A:SER:N | 1:25:A:SER:CA | 1:25:A:SER:C | 5 | 1.01 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 10 | 1.01 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 18 | 1.01 |
| (1,116) | 1:59:A:ARG:N | 1:59:A:ARG:CA | 1:59:A:ARG:C | 1:60:A:HIS:N | 6 | 1.0 |
| (1,32) | 1:17:A:LYS:N | 1:17:A:LYS:CA | 1:17:A:LYS:C | 1:18:A:LYS:N | 1 | 1.0 |