



Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 11:37 AM EST

PDB ID : 2FE0
BMRB ID : 6910
Title : NMR structure of SMP-1 (Small Myristoylated Protein) from Leishmania major
Authors : Gooley, P.R.; Mertens, H.D.T.; Tull, D.; McConville, M.J.
Deposited on : 2005-12-14

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

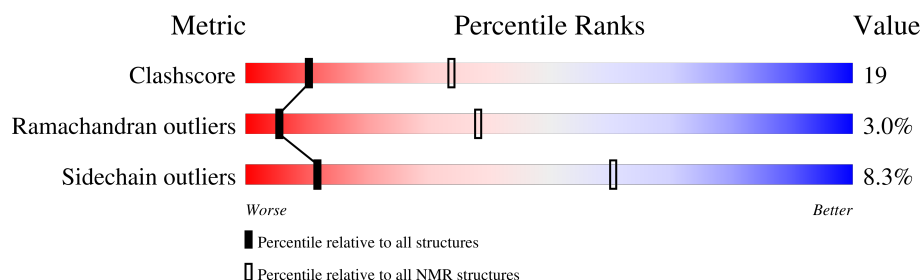
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 80%.

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 | 136 |  |

2 Ensemble composition and analysis

This entry contains 24 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues | | | |
|--------------------------------------|-----------------------|-------------------|--------------|
| Well-defined core | Residue range (total) | Backbone RMSD (Å) | Medoid model |
| 1 | A:14-A:122 (109) | 0.38 | 14 |

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

| Cluster number | Models |
|-----------------------|------------------------------------------|
| 1 | 1, 3, 10, 11, 14, 15, 19, 20, 21, 23, 24 |
| 2 | 2, 4, 5, 6, 7, 12, 13, 16, 17, 22 |
| 3 | 9, 18 |
| Single-model clusters | 8 |

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2068 atoms, of which 1016 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called small myristoylated protein 1.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|-------|
| 1 | A | 131 | Total | C | H | N | O | S | 0 |
| | | | 2068 | 660 | 1016 | 176 | 209 | 7 | |

There are 5 discrepancies between the modelled and reference sequences:

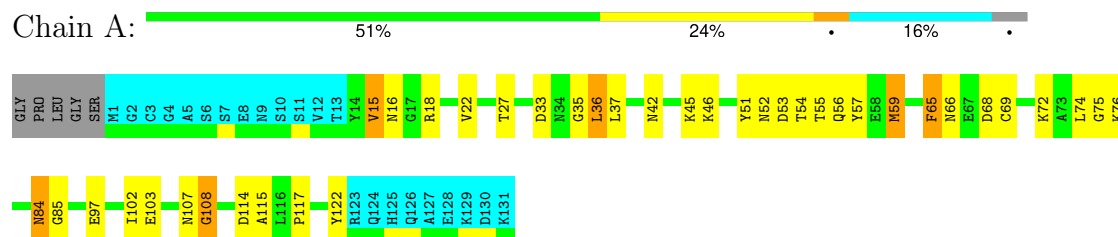
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|-------------|
| A | -4 | GLY | - | cloning artifact | GB 55714656 |
| A | -3 | PRO | - | cloning artifact | GB 55714656 |
| A | -2 | LEU | - | cloning artifact | GB 55714656 |
| A | -1 | GLY | - | cloning artifact | GB 55714656 |
| A | 0 | SER | - | cloning artifact | GB 55714656 |

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: small myristoylated protein 1

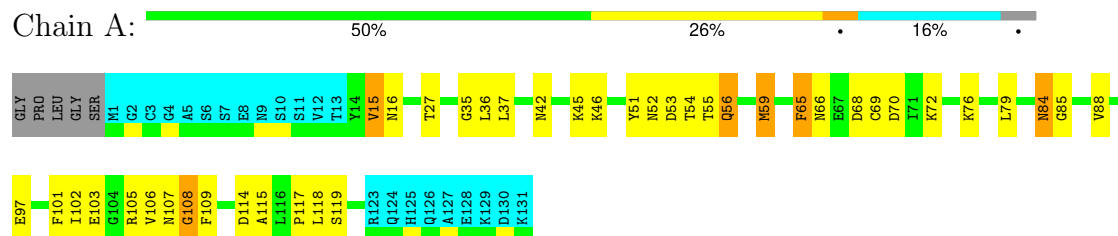


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

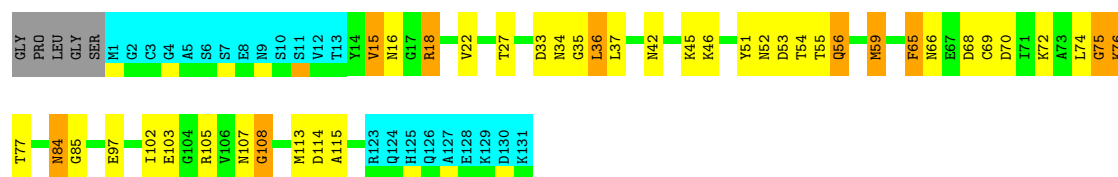
- Molecule 1: small myristoylated protein 1



4.2.2 Score per residue for model 2

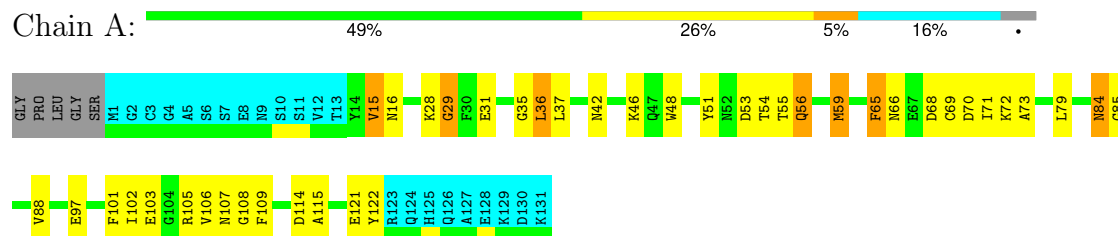
- Molecule 1: small myristoylated protein 1





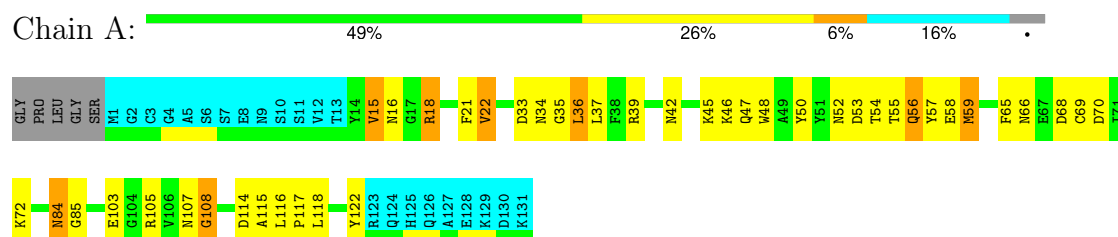
4.2.3 Score per residue for model 3

- Molecule 1: small myristoylated protein 1



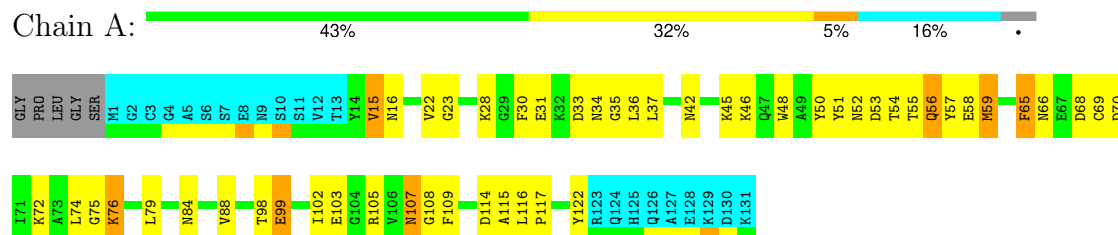
4.2.4 Score per residue for model 4

- Molecule 1: small myristoylated protein 1



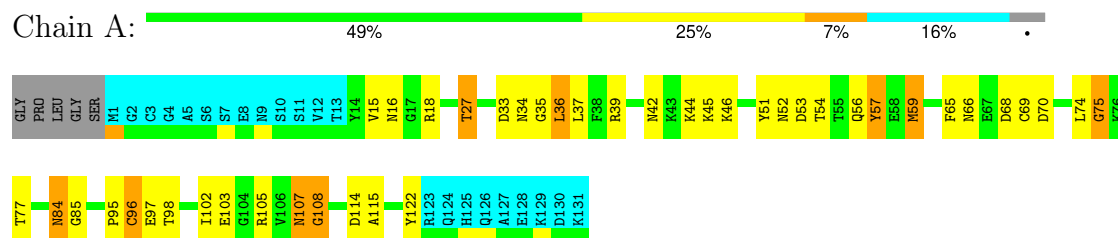
4.2.5 Score per residue for model 5

- Molecule 1: small myristoylated protein 1



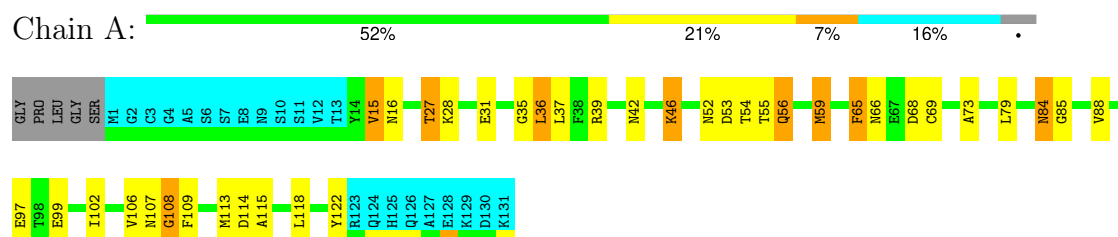
4.2.6 Score per residue for model 6

- Molecule 1: small myristoylated protein 1



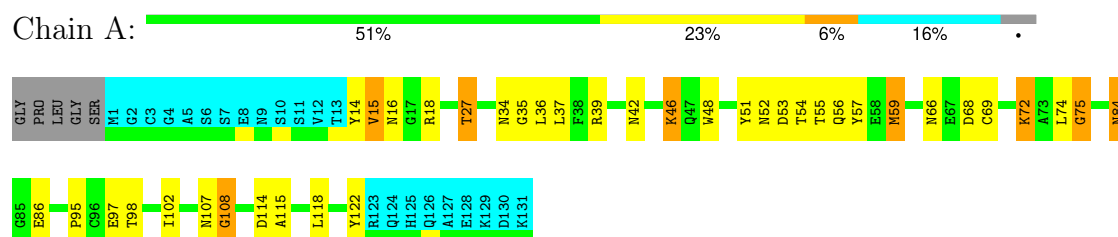
4.2.7 Score per residue for model 7

- Molecule 1: small myristoylated protein 1



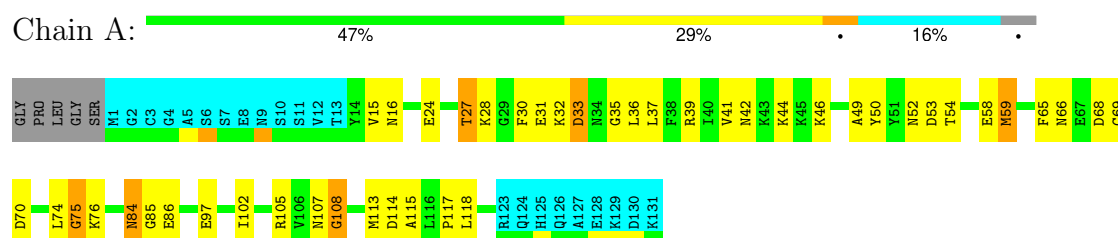
4.2.8 Score per residue for model 8

- Molecule 1: small myristoylated protein 1



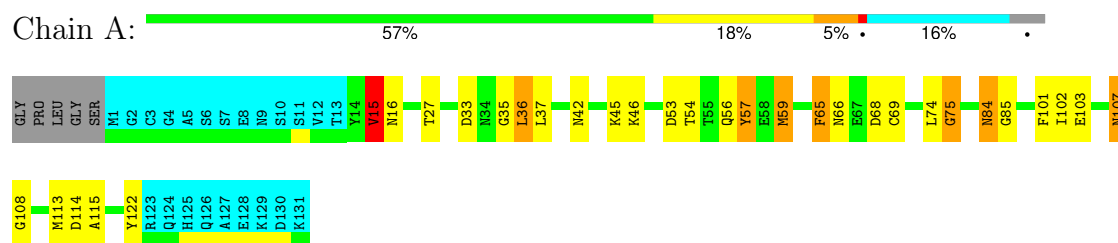
4.2.9 Score per residue for model 9

- Molecule 1: small myristoylated protein 1



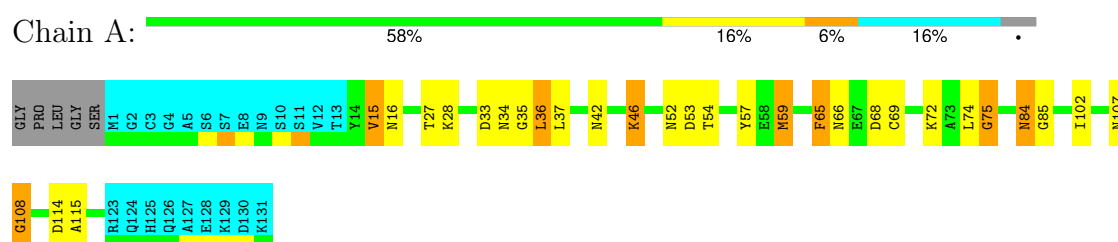
4.2.10 Score per residue for model 10

- Molecule 1: small myristoylated protein 1



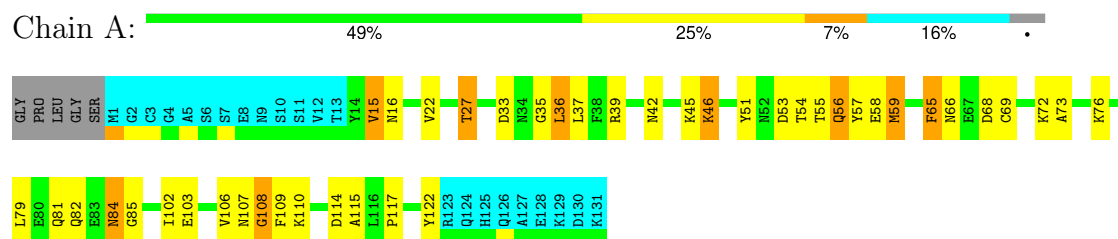
4.2.11 Score per residue for model 11

- Molecule 1: small myristoylated protein 1



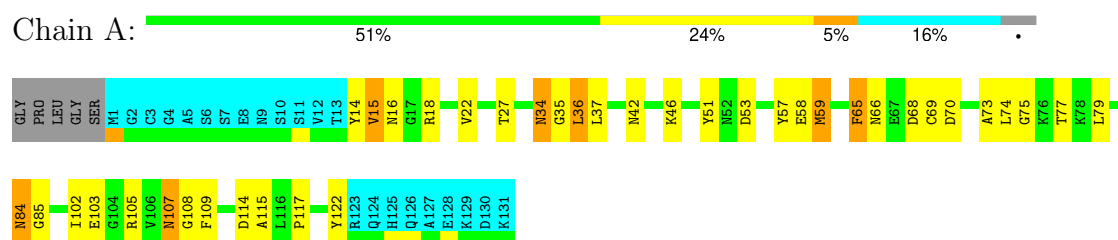
4.2.12 Score per residue for model 12

- Molecule 1: small myristoylated protein 1



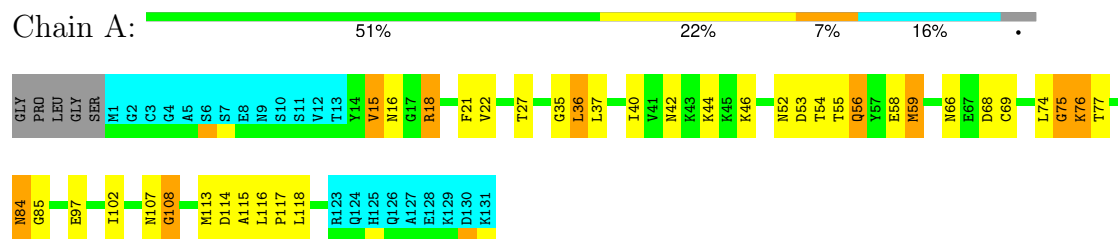
4.2.13 Score per residue for model 13

- Molecule 1: small myristoylated protein 1



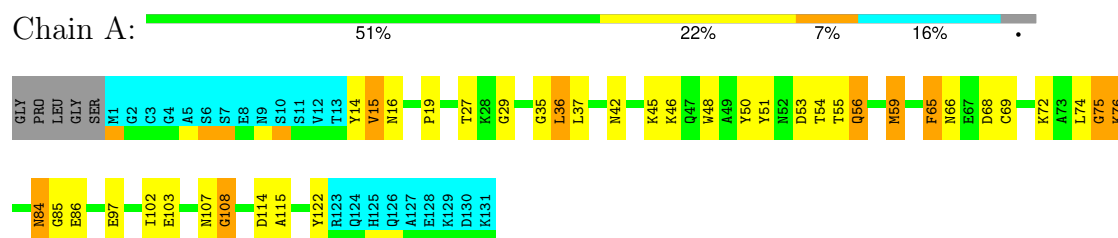
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: small myristoylated protein 1



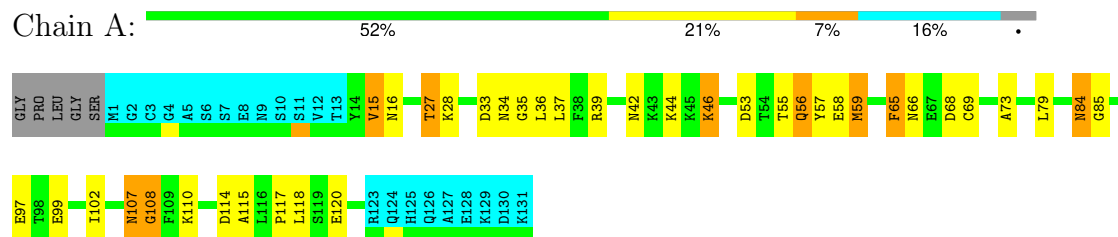
4.2.15 Score per residue for model 15

- Molecule 1: small myristoylated protein 1



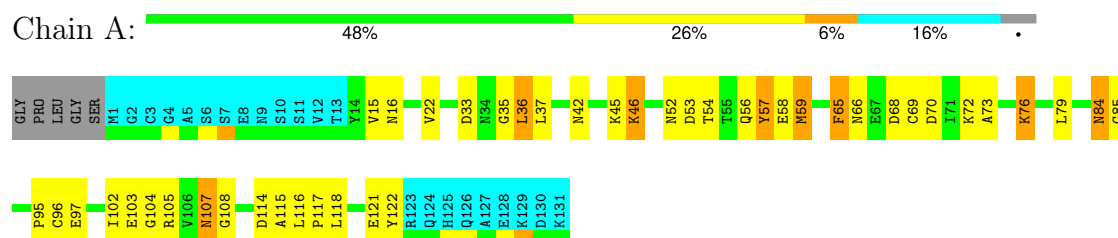
4.2.16 Score per residue for model 16

- Molecule 1: small myristoylated protein 1



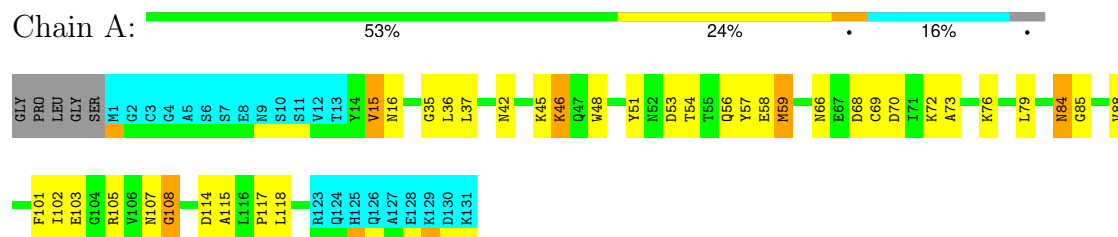
4.2.17 Score per residue for model 17

- Molecule 1: small myristoylated protein 1



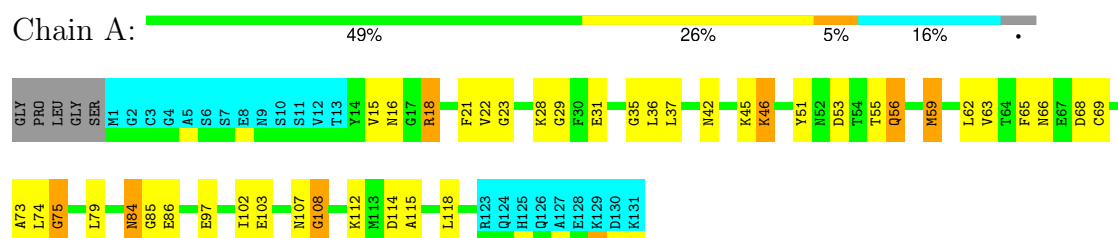
4.2.18 Score per residue for model 18

- Molecule 1: small myristoylated protein 1



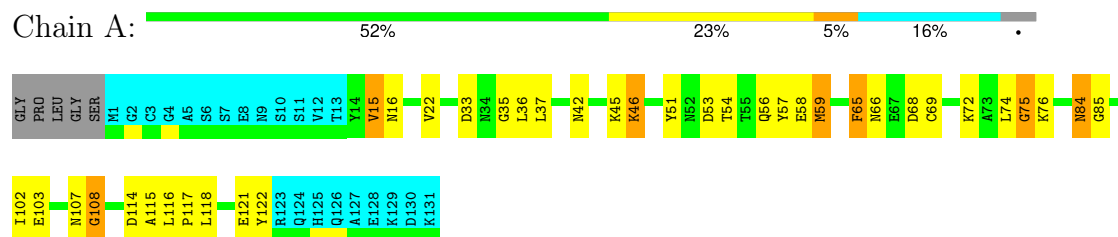
4.2.19 Score per residue for model 19

- Molecule 1: small myristoylated protein 1



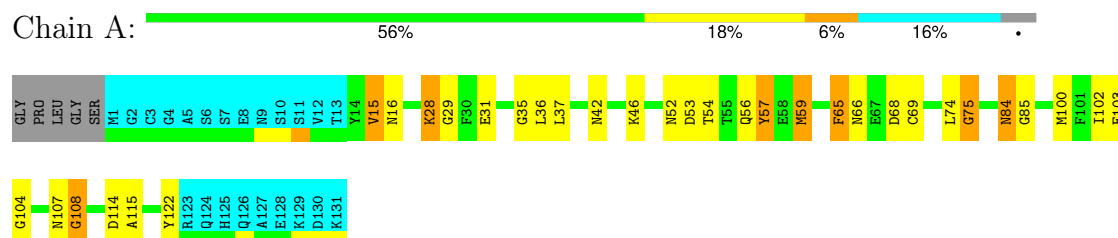
4.2.20 Score per residue for model 20

- Molecule 1: small myristoylated protein 1



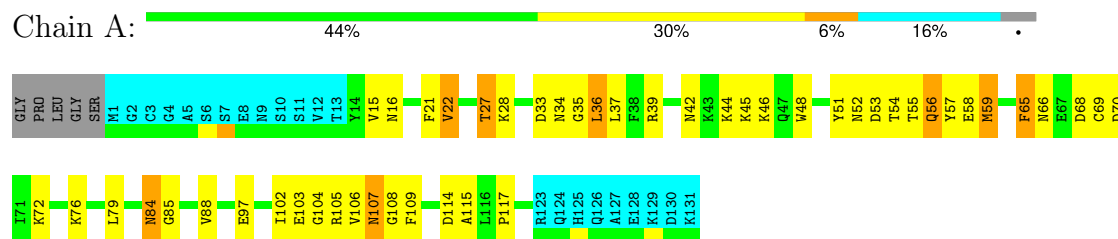
4.2.21 Score per residue for model 21

- Molecule 1: small myristoylated protein 1



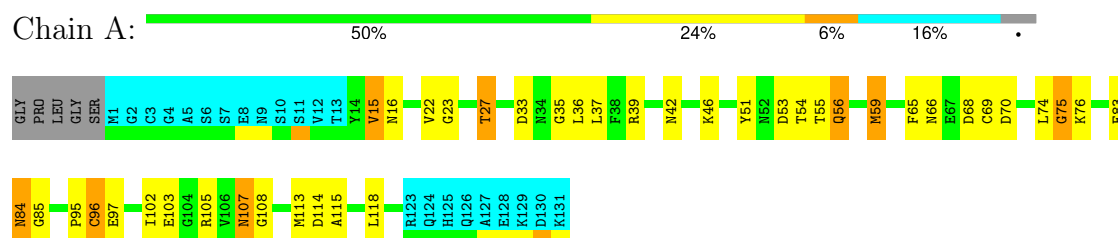
4.2.22 Score per residue for model 22

- Molecule 1: small myristoylated protein 1



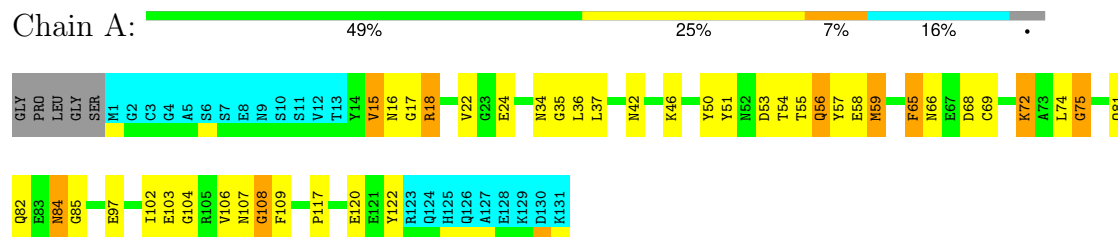
4.2.23 Score per residue for model 23

- Molecule 1: small myristoylated protein 1



4.2.24 Score per residue for model 24

- Molecule 1: small myristoylated protein 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 24 were deposited, based on the following criterion: *the smallest constraint violations, most favourable non-bond energies*.

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

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CYANA-CANDID | structure solution | 1.0.7 |
| XPLOR-NIH | refinement | 2.11 |

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 | 1386 |
| Number of shifts mapped to atoms | 1386 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 80% |

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 890 | 865 | 864 | 33±5 |
| All | All | 21360 | 20760 | 20736 | 782 |

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 19.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:102:ILE:C | 1:A:102:ILE:HD12 | 0.67 | 2.10 | 7 | 19 |
| 1:A:22:VAL:HG22 | 1:A:23:GLY:H | 0.67 | 1.50 | 19 | 3 |
| 1:A:59:MET:N | 1:A:59:MET:SD | 0.66 | 2.69 | 7 | 21 |
| 1:A:22:VAL:HG22 | 1:A:23:GLY:N | 0.66 | 2.04 | 19 | 3 |
| 1:A:42:ASN:O | 1:A:46:LYS:N | 0.66 | 2.28 | 3 | 24 |
| 1:A:39:ARG:NH1 | 1:A:50:TYR:CZ | 0.66 | 2.64 | 9 | 1 |
| 1:A:72:LYS:NZ | 1:A:72:LYS:CB | 0.64 | 2.61 | 24 | 2 |
| 1:A:18:ARG:NE | 1:A:18:ARG:N | 0.63 | 2.47 | 2 | 5 |
| 1:A:45:LYS:NZ | 1:A:47:GLN:NE2 | 0.63 | 2.47 | 4 | 1 |
| 1:A:84:ASN:HD22 | 1:A:85:GLY:N | 0.63 | 1.92 | 9 | 22 |
| 1:A:58:GLU:N | 1:A:58:GLU:OE1 | 0.62 | 2.32 | 20 | 7 |
| 1:A:39:ARG:NH1 | 1:A:50:TYR:CE2 | 0.62 | 2.68 | 9 | 1 |
| 1:A:107:ASN:N | 1:A:107:ASN:OD1 | 0.61 | 2.33 | 3 | 11 |
| 1:A:37:LEU:HD12 | 1:A:51:TYR:O | 0.61 | 1.96 | 18 | 15 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:52:ASN:ND2 | 1:A:59:MET:SD | 0.61 | 2.74 | 17 | 5 |
| 1:A:39:ARG:NH2 | 1:A:49:ALA:N | 0.60 | 2.48 | 9 | 1 |
| 1:A:14:TYR:CD1 | 1:A:18:ARG:NE | 0.60 | 2.70 | 13 | 2 |
| 1:A:69:CYS:SG | 1:A:107:ASN:ND2 | 0.60 | 2.74 | 9 | 7 |
| 1:A:55:THR:H | 1:A:56:GLN:NE2 | 0.60 | 1.95 | 7 | 8 |
| 1:A:18:ARG:HE | 1:A:18:ARG:H | 0.60 | 1.40 | 4 | 3 |
| 1:A:59:MET:SD | 1:A:59:MET:N | 0.59 | 2.75 | 9 | 3 |
| 1:A:68:ASP:O | 1:A:107:ASN:ND2 | 0.58 | 2.35 | 20 | 18 |
| 1:A:53:ASP:OD1 | 1:A:54:THR:N | 0.58 | 2.37 | 14 | 19 |
| 1:A:18:ARG:HE | 1:A:18:ARG:N | 0.58 | 1.97 | 4 | 1 |
| 1:A:72:LYS:N | 1:A:103:GLU:O | 0.57 | 2.38 | 12 | 9 |
| 1:A:18:ARG:NE | 1:A:18:ARG:H | 0.56 | 1.97 | 2 | 2 |
| 1:A:18:ARG:N | 1:A:18:ARG:HE | 0.56 | 1.98 | 19 | 2 |
| 1:A:15:VAL:HG22 | 1:A:16:ASN:N | 0.56 | 2.15 | 24 | 18 |
| 1:A:16:ASN:ND2 | 1:A:53:ASP:O | 0.56 | 2.38 | 23 | 24 |
| 1:A:31:GLU:H | 1:A:31:GLU:CD | 0.55 | 2.04 | 3 | 2 |
| 1:A:16:ASN:ND2 | 1:A:53:ASP:OD2 | 0.55 | 2.40 | 19 | 4 |
| 1:A:65:PHE:CD1 | 1:A:65:PHE:N | 0.55 | 2.75 | 24 | 16 |
| 1:A:114:ASP:OD1 | 1:A:115:ALA:N | 0.55 | 2.40 | 7 | 23 |
| 1:A:72:LYS:CB | 1:A:72:LYS:HZ3 | 0.55 | 2.15 | 8 | 2 |
| 1:A:45:LYS:HZ2 | 1:A:47:GLN:NE2 | 0.54 | 1.99 | 4 | 1 |
| 1:A:39:ARG:CZ | 1:A:50:TYR:CZ | 0.54 | 2.89 | 9 | 1 |
| 1:A:58:GLU:H | 1:A:58:GLU:CD | 0.54 | 2.05 | 12 | 4 |
| 1:A:18:ARG:N | 1:A:18:ARG:CD | 0.54 | 2.70 | 2 | 5 |
| 1:A:35:GLY:O | 1:A:37:LEU:N | 0.54 | 2.40 | 23 | 24 |
| 1:A:55:THR:N | 1:A:56:GLN:NE2 | 0.54 | 2.55 | 7 | 6 |
| 1:A:39:ARG:NH2 | 1:A:49:ALA:O | 0.54 | 2.37 | 9 | 1 |
| 1:A:84:ASN:ND2 | 1:A:86:GLU:OE1 | 0.53 | 2.36 | 8 | 1 |
| 1:A:39:ARG:NH1 | 1:A:50:TYR:OH | 0.53 | 2.41 | 4 | 1 |
| 1:A:66:ASN:O | 1:A:69:CYS:SG | 0.53 | 2.67 | 3 | 24 |
| 1:A:27:THR:O | 1:A:39:ARG:N | 0.53 | 2.41 | 22 | 8 |
| 1:A:68:ASP:O | 1:A:69:CYS:SG | 0.53 | 2.67 | 3 | 23 |
| 1:A:95:PRO:O | 1:A:97:GLU:N | 0.53 | 2.42 | 23 | 2 |
| 1:A:84:ASN:ND2 | 1:A:85:GLY:N | 0.53 | 2.56 | 3 | 21 |
| 1:A:95:PRO:O | 1:A:96:CYS:SG | 0.53 | 2.65 | 17 | 3 |
| 1:A:75:GLY:O | 1:A:77:THR:N | 0.52 | 2.39 | 13 | 2 |
| 1:A:69:CYS:SG | 1:A:107:ASN:OD1 | 0.52 | 2.68 | 3 | 3 |
| 1:A:52:ASN:OD1 | 1:A:53:ASP:N | 0.52 | 2.43 | 5 | 8 |
| 1:A:55:THR:N | 1:A:56:GLN:OE1 | 0.52 | 2.43 | 15 | 6 |
| 1:A:73:ALA:HB2 | 1:A:79:LEU:HB2 | 0.52 | 1.82 | 13 | 8 |
| 1:A:22:VAL:CG2 | 1:A:23:GLY:N | 0.51 | 2.74 | 19 | 3 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:54:THR:OG1 | 1:A:59:MET:SD | 0.51 | 2.69 | 7 | 5 |
| 1:A:21:PHE:CE2 | 1:A:22:VAL:O | 0.51 | 2.64 | 22 | 3 |
| 1:A:56:GLN:CD | 1:A:56:GLN:N | 0.51 | 2.65 | 4 | 14 |
| 1:A:34:ASN:OD1 | 1:A:35:GLY:N | 0.50 | 2.44 | 24 | 1 |
| 1:A:107:ASN:O | 1:A:108:GLY:O | 0.49 | 2.30 | 7 | 17 |
| 1:A:65:PHE:CD1 | 1:A:71:ILE:CD1 | 0.49 | 2.95 | 3 | 1 |
| 1:A:84:ASN:C | 1:A:84:ASN:ND2 | 0.49 | 2.64 | 22 | 1 |
| 1:A:69:CYS:SG | 1:A:107:ASN:O | 0.49 | 2.70 | 24 | 5 |
| 1:A:14:TYR:CE1 | 1:A:18:ARG:NH2 | 0.49 | 2.79 | 8 | 2 |
| 1:A:97:GLU:CD | 1:A:98:THR:N | 0.49 | 2.66 | 8 | 1 |
| 1:A:106:VAL:HG12 | 1:A:109:PHE:CD1 | 0.49 | 2.42 | 12 | 6 |
| 1:A:103:GLU:CD | 1:A:104:GLY:N | 0.49 | 2.66 | 22 | 3 |
| 1:A:74:LEU:O | 1:A:75:GLY:O | 0.48 | 2.31 | 21 | 13 |
| 1:A:58:GLU:OE1 | 1:A:118:LEU:HD23 | 0.48 | 2.07 | 16 | 1 |
| 1:A:95:PRO:C | 1:A:97:GLU:N | 0.48 | 2.66 | 23 | 2 |
| 1:A:83:GLU:CD | 1:A:84:ASN:N | 0.48 | 2.67 | 23 | 1 |
| 1:A:102:ILE:C | 1:A:102:ILE:CD1 | 0.48 | 2.81 | 8 | 19 |
| 1:A:58:GLU:OE2 | 1:A:117:PRO:O | 0.48 | 2.31 | 4 | 12 |
| 1:A:57:TYR:CD1 | 1:A:57:TYR:N | 0.48 | 2.80 | 11 | 1 |
| 1:A:76:LYS:CB | 1:A:76:LYS:NZ | 0.48 | 2.77 | 2 | 3 |
| 1:A:58:GLU:OE1 | 1:A:118:LEU:N | 0.48 | 2.46 | 14 | 5 |
| 1:A:56:GLN:CD | 1:A:57:TYR:CZ | 0.48 | 2.87 | 17 | 6 |
| 1:A:58:GLU:OE2 | 1:A:117:PRO:C | 0.48 | 2.52 | 22 | 3 |
| 1:A:68:ASP:C | 1:A:69:CYS:SG | 0.47 | 2.92 | 20 | 23 |
| 1:A:39:ARG:HH21 | 1:A:49:ALA:C | 0.47 | 2.12 | 9 | 1 |
| 1:A:54:THR:OG1 | 1:A:59:MET:CE | 0.47 | 2.62 | 10 | 3 |
| 1:A:63:VAL:CG1 | 1:A:65:PHE:CZ | 0.47 | 2.98 | 19 | 1 |
| 1:A:97:GLU:OE1 | 1:A:98:THR:N | 0.47 | 2.48 | 8 | 1 |
| 1:A:50:TYR:O | 1:A:99:GLU:OE2 | 0.47 | 2.33 | 5 | 1 |
| 1:A:36:LEU:O | 1:A:53:ASP:OD1 | 0.46 | 2.34 | 14 | 10 |
| 1:A:37:LEU:HD21 | 1:A:50:TYR:CD1 | 0.46 | 2.44 | 24 | 3 |
| 1:A:31:GLU:N | 1:A:31:GLU:OE1 | 0.46 | 2.46 | 21 | 1 |
| 1:A:75:GLY:C | 1:A:77:THR:N | 0.46 | 2.68 | 2 | 1 |
| 1:A:99:GLU:N | 1:A:99:GLU:CD | 0.46 | 2.68 | 5 | 1 |
| 1:A:36:LEU:O | 1:A:53:ASP:OD2 | 0.46 | 2.33 | 23 | 3 |
| 1:A:28:LYS:O | 1:A:29:GLY:C | 0.46 | 2.53 | 3 | 3 |
| 1:A:107:ASN:O | 1:A:107:ASN:OD1 | 0.46 | 2.34 | 9 | 6 |
| 1:A:81:GLN:C | 1:A:82:GLN:NE2 | 0.46 | 2.69 | 24 | 2 |
| 1:A:28:LYS:NZ | 1:A:31:GLU:OE1 | 0.46 | 2.42 | 19 | 1 |
| 1:A:113:MET:SD | 1:A:113:MET:N | 0.46 | 2.89 | 7 | 6 |
| 1:A:70:ASP:O | 1:A:105:ARG:N | 0.46 | 2.49 | 5 | 12 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:75:GLY:C | 1:A:77:THR:H | 0.45 | 2.14 | 2 | 3 |
| 1:A:31:GLU:CD | 1:A:31:GLU:N | 0.45 | 2.70 | 3 | 1 |
| 1:A:68:ASP:O | 1:A:68:ASP:OD1 | 0.45 | 2.35 | 13 | 3 |
| 1:A:107:ASN:OD1 | 1:A:107:ASN:O | 0.45 | 2.35 | 8 | 1 |
| 1:A:52:ASN:OD1 | 1:A:54:THR:O | 0.45 | 2.34 | 1 | 2 |
| 1:A:48:TRP:N | 1:A:48:TRP:CD1 | 0.45 | 2.85 | 18 | 7 |
| 1:A:33:ASP:CG | 1:A:34:ASN:H | 0.45 | 2.15 | 4 | 6 |
| 1:A:39:ARG:CZ | 1:A:50:TYR:CE2 | 0.45 | 3.00 | 9 | 1 |
| 1:A:45:LYS:O | 1:A:103:GLU:OE2 | 0.44 | 2.35 | 20 | 12 |
| 1:A:74:LEU:HD21 | 1:A:103:GLU:CD | 0.44 | 2.33 | 23 | 2 |
| 1:A:14:TYR:CE2 | 1:A:19:PRO:CD | 0.44 | 3.00 | 15 | 1 |
| 1:A:121:GLU:CG | 1:A:122:TYR:N | 0.44 | 2.80 | 17 | 2 |
| 1:A:22:VAL:CG2 | 1:A:23:GLY:H | 0.44 | 2.21 | 19 | 3 |
| 1:A:17:GLY:O | 1:A:51:TYR:OH | 0.44 | 2.36 | 24 | 1 |
| 1:A:65:PHE:O | 1:A:86:GLU:OE1 | 0.43 | 2.36 | 9 | 2 |
| 1:A:109:PHE:CD1 | 1:A:109:PHE:N | 0.43 | 2.86 | 3 | 5 |
| 1:A:66:ASN:HD22 | 1:A:68:ASP:CG | 0.43 | 2.16 | 14 | 3 |
| 1:A:34:ASN:ND2 | 1:A:53:ASP:OD2 | 0.43 | 2.43 | 2 | 1 |
| 1:A:72:LYS:HZ3 | 1:A:72:LYS:HB3 | 0.43 | 1.72 | 8 | 1 |
| 1:A:32:LYS:O | 1:A:33:ASP:O | 0.43 | 2.36 | 9 | 1 |
| 1:A:79:LEU:HD12 | 1:A:88:VAL:O | 0.43 | 2.12 | 3 | 6 |
| 1:A:58:GLU:CD | 1:A:116:LEU:O | 0.43 | 2.56 | 20 | 4 |
| 1:A:84:ASN:ND2 | 1:A:86:GLU:N | 0.43 | 2.67 | 19 | 1 |
| 1:A:39:ARG:NH2 | 1:A:49:ALA:C | 0.43 | 2.72 | 9 | 1 |
| 1:A:33:ASP:CB | 1:A:36:LEU:HD21 | 0.43 | 2.43 | 23 | 1 |
| 1:A:56:GLN:CG | 1:A:57:TYR:CE2 | 0.43 | 3.02 | 18 | 5 |
| 1:A:18:ARG:H | 1:A:18:ARG:HE | 0.43 | 1.57 | 2 | 1 |
| 1:A:44:LYS:NZ | 1:A:45:LYS:NZ | 0.43 | 2.67 | 22 | 1 |
| 1:A:84:ASN:HD22 | 1:A:84:ASN:C | 0.42 | 2.15 | 22 | 1 |
| 1:A:97:GLU:OE2 | 1:A:99:GLU:OE2 | 0.42 | 2.37 | 16 | 2 |
| 1:A:24:GLU:OE1 | 1:A:24:GLU:C | 0.42 | 2.58 | 24 | 1 |
| 1:A:68:ASP:C | 1:A:69:CYS:HG | 0.42 | 2.17 | 10 | 2 |
| 1:A:24:GLU:N | 1:A:41:VAL:O | 0.42 | 2.49 | 9 | 1 |
| 1:A:103:GLU:CG | 1:A:104:GLY:N | 0.42 | 2.81 | 21 | 4 |
| 1:A:37:LEU:HD13 | 1:A:59:MET:HG2 | 0.42 | 1.92 | 18 | 1 |
| 1:A:58:GLU:N | 1:A:116:LEU:O | 0.42 | 2.51 | 5 | 1 |
| 1:A:74:LEU:O | 1:A:75:GLY:C | 0.41 | 2.59 | 5 | 1 |
| 1:A:34:ASN:C | 1:A:36:LEU:H | 0.41 | 2.18 | 11 | 2 |
| 1:A:107:ASN:O | 1:A:107:ASN:CG | 0.41 | 2.59 | 9 | 4 |
| 1:A:101:PHE:CG | 1:A:102:ILE:N | 0.41 | 2.84 | 1 | 4 |
| 1:A:118:LEU:HD13 | 1:A:122:TYR:CE2 | 0.41 | 2.50 | 7 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|-----------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:33:ASP:C | 1:A:35:GLY:H | 0.41 | 2.19 | 11 | 1 |
| 1:A:58:GLU:OE1 | 1:A:118:LEU:CD2 | 0.41 | 2.68 | 16 | 1 |
| 1:A:52:ASN:OD1 | 1:A:52:ASN:C | 0.41 | 2.59 | 1 | 1 |
| 1:A:117:PRO:O | 1:A:119:SER:N | 0.41 | 2.54 | 1 | 1 |
| 1:A:18:ARG:H | 1:A:18:ARG:NE | 0.41 | 2.06 | 4 | 1 |
| 1:A:56:GLN:O | 1:A:57:TYR:CD1 | 0.41 | 2.74 | 22 | 3 |
| 1:A:76:LYS:NZ | 1:A:76:LYS:CB | 0.41 | 2.84 | 14 | 2 |
| 1:A:120:GLU:OE1 | 1:A:120:GLU:C | 0.40 | 2.60 | 24 | 1 |
| 1:A:31:GLU:OE1 | 1:A:31:GLU:N | 0.40 | 2.51 | 7 | 1 |
| 1:A:55:THR:O | 1:A:118:LEU:CD1 | 0.40 | 2.70 | 8 | 1 |
| 1:A:21:PHE:O | 1:A:40:ILE:HD13 | 0.40 | 2.17 | 14 | 1 |
| 1:A:102:ILE:HD12 | 1:A:103:GLU:N | 0.40 | 2.32 | 13 | 1 |
| 1:A:62:LEU:HD23 | 1:A:112:LYS:NZ | 0.40 | 2.31 | 19 | 1 |

6.3 Torsion angles

6.3.1 Protein backbone

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|-------------|------------|-------------|----|
| 1 | A | 109/136 (80%) | 96±2 (88±2%) | 10±2 (9±1%) | 3±1 (3±1%) | 5 | 38 |
| All | All | 2616/3264 (80%) | 2293 (88%) | 244 (9%) | 79 (3%) | 5 | 38 |

All 11 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 | 108 | GLY | 24 |
| 1 | A | 36 | LEU | 22 |
| 1 | A | 75 | GLY | 13 |
| 1 | A | 118 | LEU | 5 |
| 1 | A | 33 | ASP | 5 |
| 1 | A | 15 | VAL | 2 |
| 1 | A | 29 | GLY | 2 |
| 1 | A | 30 | PHE | 2 |
| 1 | A | 96 | CYS | 2 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 31 | GLU | 1 |
| 1 | A | 95 | PRO | 1 |

6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|--------------|------------|-------------|----|
| 1 | A | 97/118 (82%) | 89±2 (92±2%) | 8±2 (8±2%) | 12 | 60 |
| All | All | 2328/2832 (82%) | 2135 (92%) | 193 (8%) | 12 | 60 |

All 22 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 | 15 | VAL | 24 |
| 1 | A | 59 | MET | 24 |
| 1 | A | 84 | ASN | 24 |
| 1 | A | 65 | PHE | 18 |
| 1 | A | 27 | THR | 15 |
| 1 | A | 56 | GLN | 14 |
| 1 | A | 76 | LYS | 12 |
| 1 | A | 22 | VAL | 9 |
| 1 | A | 46 | LYS | 9 |
| 1 | A | 107 | ASN | 8 |
| 1 | A | 28 | LYS | 7 |
| 1 | A | 18 | ARG | 6 |
| 1 | A | 57 | TYR | 5 |
| 1 | A | 72 | LYS | 5 |
| 1 | A | 44 | LYS | 4 |
| 1 | A | 98 | THR | 2 |
| 1 | A | 110 | LYS | 2 |
| 1 | A | 99 | GLU | 1 |
| 1 | A | 31 | GLU | 1 |
| 1 | A | 34 | ASN | 1 |
| 1 | A | 121 | GLU | 1 |
| 1 | A | 100 | MET | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 78% 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 | 1386 |
| Number of shifts mapped to atoms | 1386 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Number of shift outliers (ShiftChecker) | 6 |

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 131 | -0.03 ± 0.15 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 121 | -0.29 ± 0.20 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 0 | — | None (insufficient data) |
| ^{15}N | 125 | -0.89 ± 0.44 | Should be applied |

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 80%, i.e. 1202 atoms were assigned a chemical shift out of a possible 1505. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone | 435/547 (80%) | 222/223 (100%) | 109/218 (50%) | 104/106 (98%) |
| Sidechain | 674/812 (83%) | 442/521 (85%) | 222/260 (85%) | 10/31 (32%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 93/146 (64%) | 57/70 (81%) | 34/72 (47%) | 2/4 (50%) |
| Overall | 1202/1505 (80%) | 721/814 (89%) | 365/550 (66%) | 116/141 (82%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1385 atoms were assigned a chemical shift out of a possible 1766. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone | 516/659 (78%) | 260/269 (97%) | 131/262 (50%) | 125/128 (98%) |
| Sidechain | 772/953 (81%) | 504/610 (83%) | 256/304 (84%) | 12/39 (31%) |
| Aromatic | 97/154 (63%) | 59/74 (80%) | 36/74 (49%) | 2/6 (33%) |
| Overall | 1385/1766 (78%) | 823/953 (86%) | 423/640 (66%) | 139/173 (80%) |

7.1.4 Statistically unusual chemical shifts [i](#)

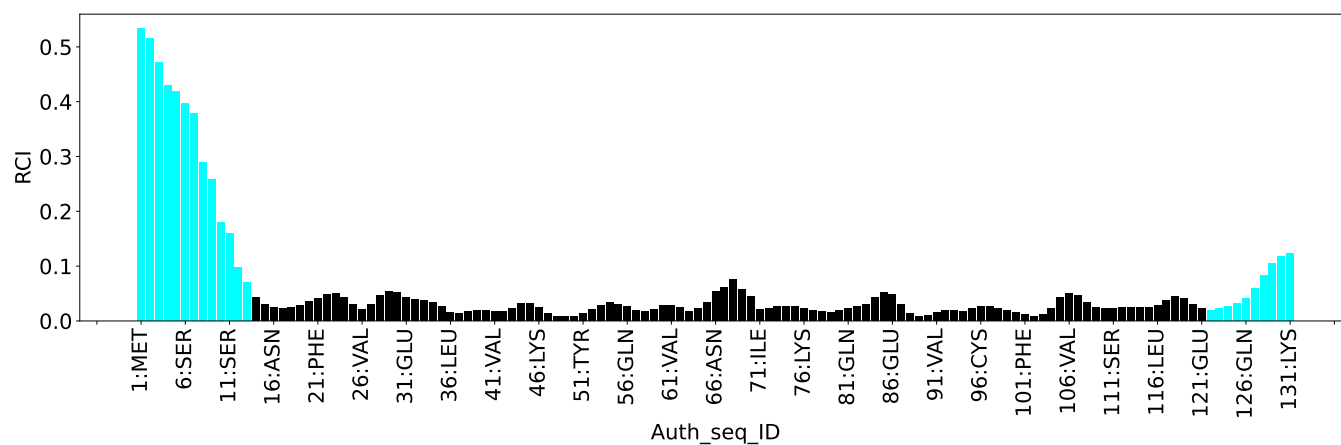
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 98 | THR | HG1 | 5.99 | 0.08 – 2.19 | 23.0 |
| 1 | A | 81 | GLN | HB2 | -0.12 | 0.80 – 3.29 | -8.7 |
| 1 | A | 19 | PRO | HD2 | 1.54 | 1.93 – 5.38 | -6.1 |
| 1 | A | 81 | GLN | HG3 | 0.64 | 0.91 – 3.68 | -6.0 |
| 1 | A | 48 | TRP | HH2 | 5.17 | 5.24 – 8.73 | -5.2 |
| 1 | A | 15 | VAL | H | 11.66 | 4.98 – 11.56 | 5.2 |

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

| Description | Value |
|----------------------------------------------------------|-------|
| Total distance restraints | 1671 |
| Intra-residue ($ i-j =0$) | 72 |
| Sequential ($ i-j =1$) | 551 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 232 |
| Long range ($ i-j \geq 5$) | 816 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 0 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 198 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 13.7 |
| Number of long range restraints per residue ¹ | 6.0 |

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) | 43.4 | 0.2 |
| 0.2-0.5 (Medium) | 5.2 | 0.27 |
| >0.5 (Large) | 0.5 | 1.61 |

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) | 4.1 | 2.69 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis ⓘ

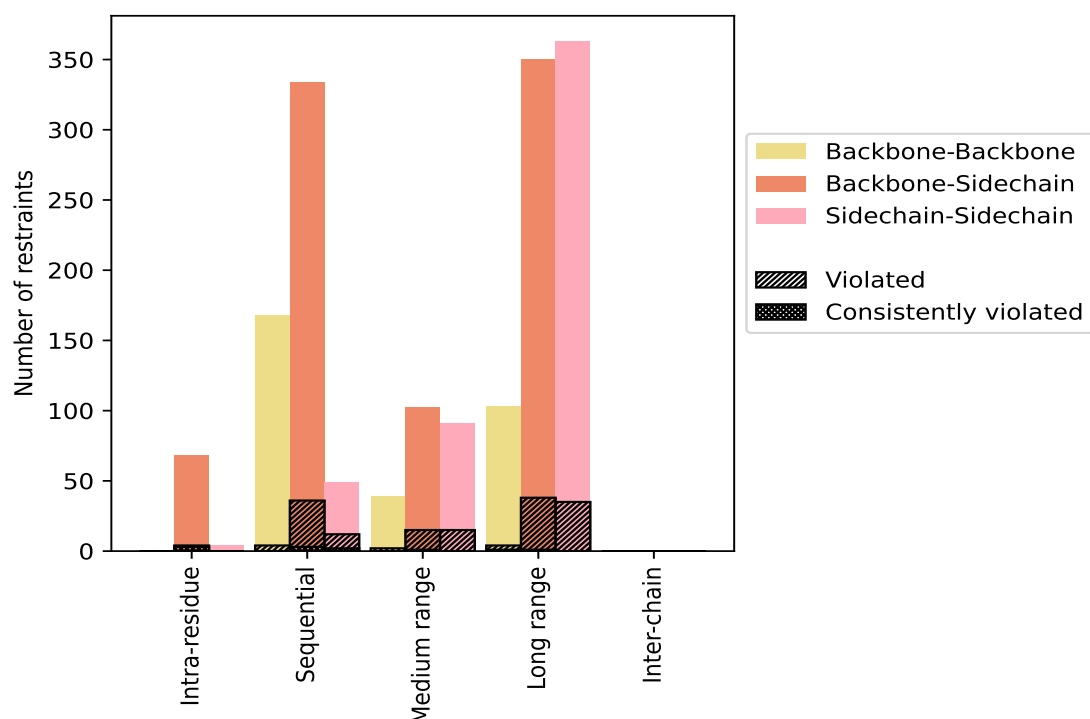
9.1 Summary of distance violations ⓘ

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|----------------------------------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($ i-j =0$) | 72 | 4.3 | 4 | 5.6 | 0.2 | 3 | 4.2 | 0.2 |
| Backbone-Backbone | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 68 | 4.1 | 4 | 5.9 | 0.2 | 3 | 4.4 | 0.2 |
| Sidechain-Sidechain | 4 | 0.2 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Sequential ($ i-j =1$) | 551 | 33.0 | 52 | 9.4 | 3.1 | 5 | 0.9 | 0.3 |
| Backbone-Backbone | 168 | 10.1 | 4 | 2.4 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 334 | 20.0 | 36 | 10.8 | 2.2 | 3 | 0.9 | 0.2 |
| Sidechain-Sidechain | 49 | 2.9 | 12 | 24.5 | 0.7 | 2 | 4.1 | 0.1 |
| Medium range ($ i-j >1$ & $ i-j <5$) | 232 | 13.9 | 32 | 13.8 | 1.9 | 1 | 0.4 | 0.1 |
| Backbone-Backbone | 39 | 2.3 | 2 | 5.1 | 0.1 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 102 | 6.1 | 15 | 14.7 | 0.9 | 1 | 1.0 | 0.1 |
| Sidechain-Sidechain | 91 | 5.4 | 15 | 16.5 | 0.9 | 0 | 0.0 | 0.0 |
| Long range ($ i-j \geq 5$) | 816 | 48.8 | 77 | 9.4 | 4.6 | 2 | 0.2 | 0.1 |
| Backbone-Backbone | 103 | 6.2 | 4 | 3.9 | 0.2 | 1 | 1.0 | 0.1 |
| Backbone-Sidechain | 350 | 20.9 | 38 | 10.9 | 2.3 | 1 | 0.3 | 0.1 |
| Sidechain-Sidechain | 363 | 21.7 | 35 | 9.6 | 2.1 | 0 | 0.0 | 0.0 |
| 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 | 1671 | 100.0 | 165 | 9.9 | 9.9 | 11 | 0.7 | 0.7 |
| Backbone-Backbone | 310 | 18.6 | 10 | 3.2 | 0.6 | 1 | 0.3 | 0.1 |
| Backbone-Sidechain | 854 | 51.1 | 93 | 10.9 | 5.6 | 8 | 0.9 | 0.5 |
| Sidechain-Sidechain | 507 | 30.3 | 62 | 12.2 | 3.7 | 2 | 0.4 | 0.1 |

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

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



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

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 3 | 21 | 7 | 19 | 0 | 50 | 0.18 | 1.61 | 0.21 | 0.15 |
| 2 | 4 | 20 | 8 | 22 | 0 | 54 | 0.17 | 1.52 | 0.19 | 0.14 |
| 3 | 4 | 19 | 6 | 27 | 0 | 56 | 0.14 | 0.26 | 0.03 | 0.13 |
| 4 | 4 | 19 | 6 | 29 | 0 | 58 | 0.18 | 1.57 | 0.19 | 0.14 |
| 5 | 4 | 13 | 7 | 22 | 0 | 46 | 0.14 | 0.23 | 0.03 | 0.14 |
| 6 | 4 | 20 | 8 | 18 | 0 | 50 | 0.17 | 1.33 | 0.17 | 0.14 |
| 7 | 4 | 21 | 8 | 23 | 0 | 56 | 0.17 | 1.46 | 0.18 | 0.15 |
| 8 | 4 | 21 | 8 | 23 | 0 | 56 | 0.15 | 0.26 | 0.03 | 0.15 |
| 9 | 4 | 21 | 7 | 22 | 0 | 54 | 0.15 | 0.25 | 0.04 | 0.14 |
| 10 | 4 | 16 | 6 | 19 | 0 | 45 | 0.18 | 1.33 | 0.18 | 0.14 |

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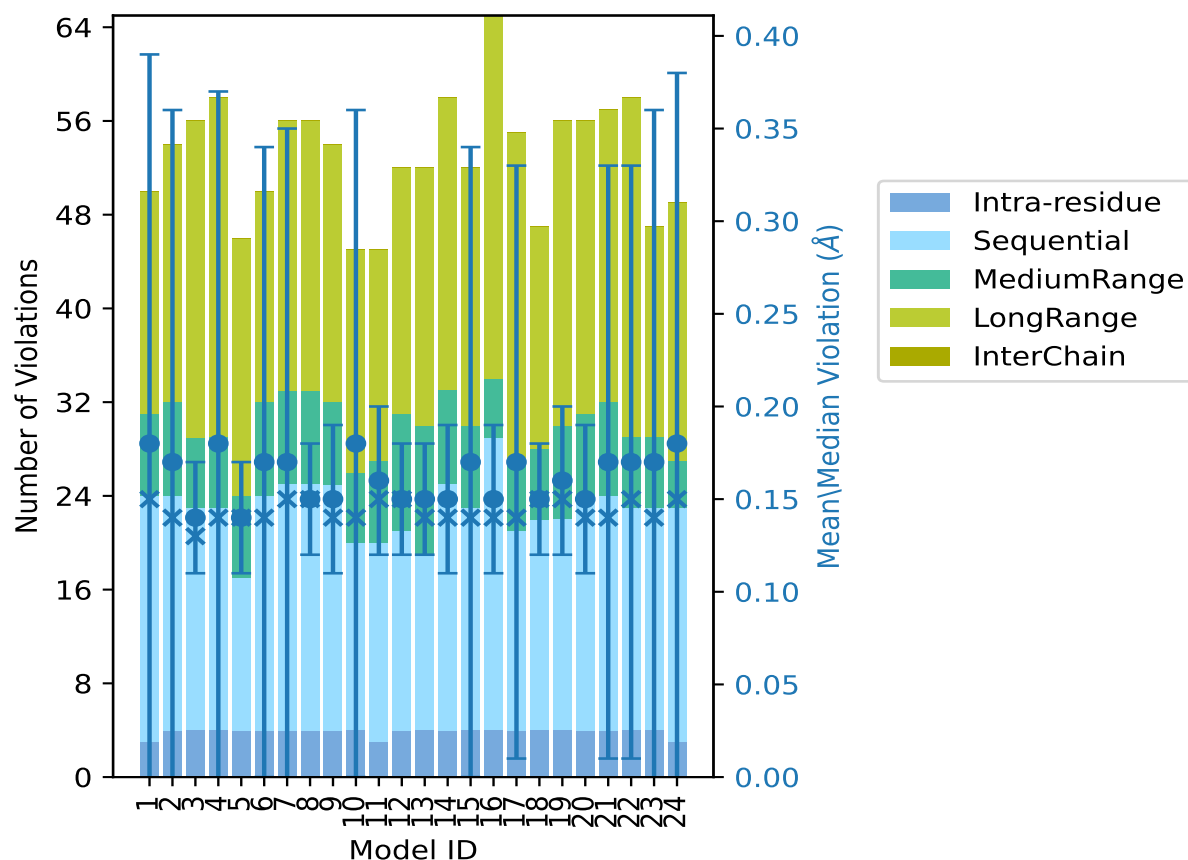
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| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 11 | 3 | 17 | 7 | 18 | 0 | 45 | 0.16 | 0.26 | 0.04 | 0.15 |
| 12 | 4 | 17 | 10 | 21 | 0 | 52 | 0.15 | 0.24 | 0.03 | 0.15 |
| 13 | 4 | 15 | 11 | 22 | 0 | 52 | 0.15 | 0.22 | 0.03 | 0.14 |
| 14 | 4 | 21 | 8 | 25 | 0 | 58 | 0.15 | 0.26 | 0.04 | 0.14 |
| 15 | 4 | 19 | 7 | 22 | 0 | 52 | 0.17 | 1.35 | 0.17 | 0.14 |
| 16 | 4 | 25 | 5 | 31 | 0 | 65 | 0.15 | 0.25 | 0.04 | 0.14 |
| 17 | 4 | 17 | 6 | 28 | 0 | 55 | 0.17 | 1.32 | 0.16 | 0.14 |
| 18 | 4 | 18 | 6 | 19 | 0 | 47 | 0.15 | 0.25 | 0.03 | 0.15 |
| 19 | 4 | 18 | 8 | 26 | 0 | 56 | 0.16 | 0.26 | 0.04 | 0.15 |
| 20 | 4 | 20 | 7 | 25 | 0 | 56 | 0.15 | 0.25 | 0.04 | 0.14 |
| 21 | 4 | 20 | 8 | 25 | 0 | 57 | 0.17 | 1.32 | 0.16 | 0.14 |
| 22 | 4 | 19 | 6 | 29 | 0 | 58 | 0.17 | 1.37 | 0.16 | 0.15 |
| 23 | 4 | 19 | 6 | 18 | 0 | 47 | 0.17 | 1.43 | 0.19 | 0.14 |
| 24 | 3 | 20 | 4 | 22 | 0 | 49 | 0.18 | 1.51 | 0.2 | 0.15 |

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



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

9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1506(IR:68, SQ:499, MR:200, LR:739, 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 | % |
| 0 | 10 | 10 | 17 | 0 | 37 | 1 | 4.2 |
| 0 | 2 | 6 | 6 | 0 | 14 | 2 | 8.3 |
| 0 | 5 | 2 | 7 | 0 | 14 | 3 | 12.5 |
| 0 | 6 | 3 | 7 | 0 | 16 | 4 | 16.7 |
| 0 | 5 | 1 | 5 | 0 | 11 | 5 | 20.8 |
| 0 | 1 | 2 | 4 | 0 | 7 | 6 | 25.0 |

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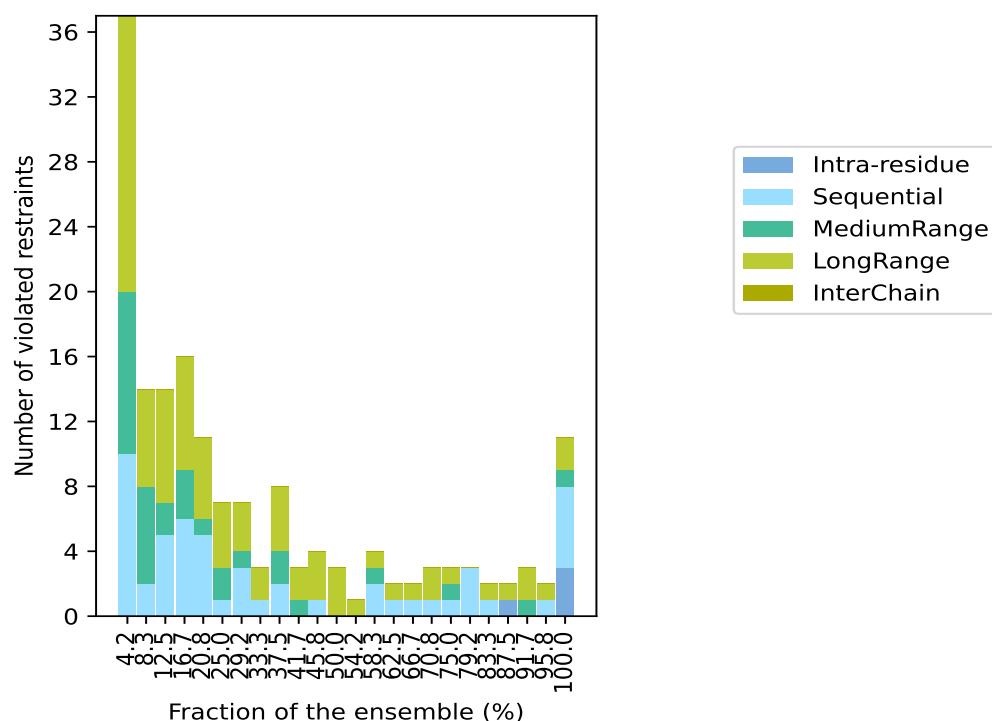
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| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 0 | 3 | 1 | 3 | 0 | 7 | 7 | 29.2 |
| 0 | 1 | 0 | 2 | 0 | 3 | 8 | 33.3 |
| 0 | 2 | 2 | 4 | 0 | 8 | 9 | 37.5 |
| 0 | 0 | 1 | 2 | 0 | 3 | 10 | 41.7 |
| 0 | 1 | 0 | 3 | 0 | 4 | 11 | 45.8 |
| 0 | 0 | 0 | 3 | 0 | 3 | 12 | 50.0 |
| 0 | 0 | 0 | 1 | 0 | 1 | 13 | 54.2 |
| 0 | 2 | 1 | 1 | 0 | 4 | 14 | 58.3 |
| 0 | 1 | 0 | 1 | 0 | 2 | 15 | 62.5 |
| 0 | 1 | 0 | 1 | 0 | 2 | 16 | 66.7 |
| 0 | 1 | 0 | 2 | 0 | 3 | 17 | 70.8 |
| 0 | 1 | 1 | 1 | 0 | 3 | 18 | 75.0 |
| 0 | 3 | 0 | 0 | 0 | 3 | 19 | 79.2 |
| 0 | 1 | 0 | 1 | 0 | 2 | 20 | 83.3 |
| 1 | 0 | 0 | 1 | 0 | 2 | 21 | 87.5 |
| 0 | 0 | 1 | 2 | 0 | 3 | 22 | 91.7 |
| 0 | 1 | 0 | 1 | 0 | 2 | 23 | 95.8 |
| 3 | 5 | 1 | 2 | 0 | 11 | 24 | 100.0 |

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

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

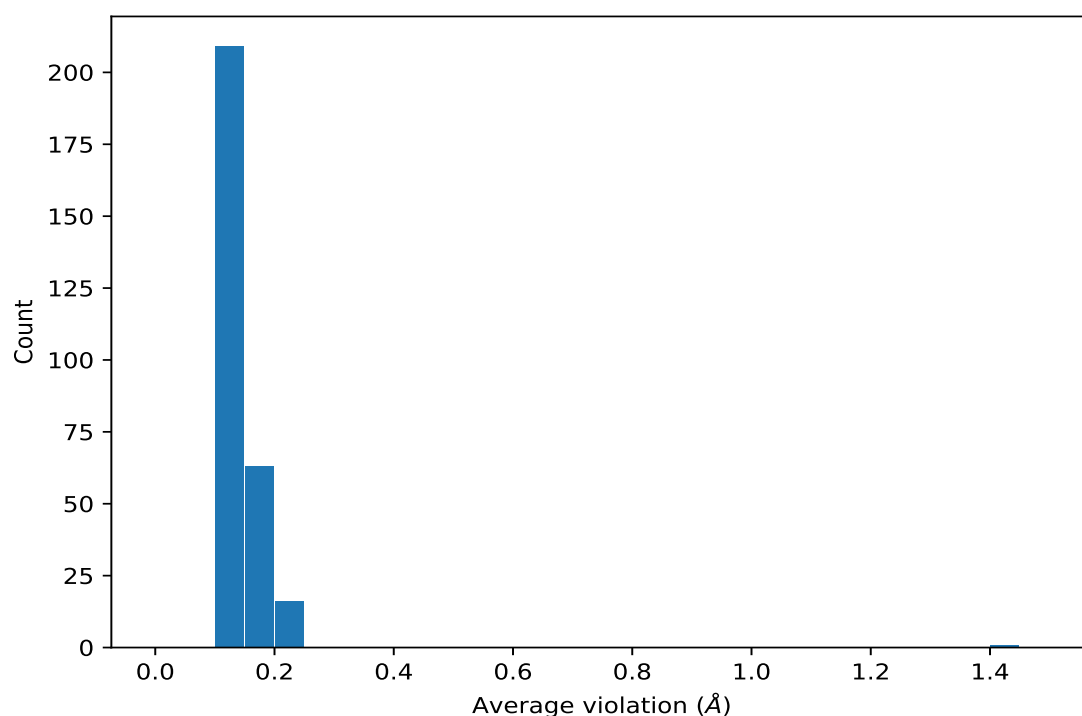
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 24 | 0.2 | 0.03 | 0.2 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 24 | 0.2 | 0.03 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 24 | 0.2 | 0.01 | 0.2 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 24 | 0.19 | 0.04 | 0.19 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 24 | 0.19 | 0.04 | 0.19 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 24 | 0.19 | 0.04 | 0.19 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 24 | 0.17 | 0.02 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 24 | 0.17 | 0.02 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 24 | 0.17 | 0.02 | 0.17 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 24 | 0.17 | 0.02 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 24 | 0.17 | 0.02 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 24 | 0.17 | 0.02 | 0.18 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 24 | 0.17 | 0.02 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 24 | 0.16 | 0.02 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 24 | 0.16 | 0.02 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 24 | 0.16 | 0.02 | 0.16 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 24 | 0.16 | 0.01 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 24 | 0.16 | 0.01 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 24 | 0.16 | 0.01 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 24 | 0.16 | 0.01 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 24 | 0.16 | 0.01 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 24 | 0.16 | 0.01 | 0.16 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 24 | 0.15 | 0.01 | 0.14 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 23 | 0.18 | 0.04 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 23 | 0.18 | 0.04 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 23 | 0.18 | 0.04 | 0.18 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 23 | 0.15 | 0.02 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 22 | 0.17 | 0.03 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 22 | 0.17 | 0.03 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 22 | 0.17 | 0.03 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 22 | 0.17 | 0.03 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 22 | 0.17 | 0.03 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 22 | 0.17 | 0.03 | 0.16 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 22 | 0.13 | 0.02 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 22 | 0.13 | 0.02 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 22 | 0.13 | 0.02 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 22 | 0.13 | 0.02 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 22 | 0.13 | 0.02 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 22 | 0.13 | 0.02 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 22 | 0.13 | 0.02 | 0.13 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 21 | 0.15 | 0.02 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 21 | 0.15 | 0.02 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 21 | 0.15 | 0.02 | 0.15 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 21 | 0.13 | 0.02 | 0.13 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 20 | 0.19 | 0.02 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 20 | 0.19 | 0.02 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 20 | 0.19 | 0.02 | 0.2 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 20 | 0.15 | 0.03 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 20 | 0.15 | 0.03 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 20 | 0.15 | 0.03 | 0.16 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 19 | 0.19 | 0.05 | 0.18 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 19 | 0.15 | 0.04 | 0.13 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 19 | 0.15 | 0.0 | 0.15 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 18 | 0.16 | 0.06 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 18 | 0.16 | 0.06 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 18 | 0.16 | 0.06 | 0.13 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 18 | 0.13 | 0.03 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 18 | 0.13 | 0.03 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 18 | 0.13 | 0.02 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 18 | 0.13 | 0.02 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 18 | 0.13 | 0.02 | 0.12 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 17 | 0.16 | 0.03 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 17 | 0.16 | 0.03 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 17 | 0.16 | 0.03 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 17 | 0.16 | 0.03 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 17 | 0.16 | 0.03 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 17 | 0.16 | 0.03 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 17 | 0.15 | 0.03 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 17 | 0.15 | 0.03 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 17 | 0.15 | 0.03 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 17 | 0.14 | 0.01 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 17 | 0.14 | 0.01 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 17 | 0.14 | 0.01 | 0.14 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 16 | 0.15 | 0.02 | 0.15 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 16 | 0.13 | 0.02 | 0.12 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 15 | 0.13 | 0.02 | 0.13 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 15 | 0.13 | 0.02 | 0.13 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 15 | 0.13 | 0.02 | 0.13 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 15 | 0.11 | 0.01 | 0.11 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 14 | 0.16 | 0.05 | 0.14 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 14 | 0.13 | 0.01 | 0.14 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 14 | 0.13 | 0.01 | 0.14 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 14 | 0.13 | 0.01 | 0.14 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 14 | 0.13 | 0.02 | 0.12 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 14 | 0.13 | 0.02 | 0.12 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 14 | 0.12 | 0.02 | 0.12 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 14 | 0.12 | 0.02 | 0.12 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 14 | 0.12 | 0.02 | 0.12 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 13 | 0.12 | 0.02 | 0.12 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 12 | 1.43 | 0.1 | 1.4 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 12 | 0.19 | 0.03 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 12 | 0.19 | 0.03 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 12 | 0.19 | 0.03 | 0.18 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 12 | 0.15 | 0.02 | 0.15 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 12 | 0.15 | 0.02 | 0.15 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 11 | 0.15 | 0.02 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 11 | 0.14 | 0.01 | 0.14 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 11 | 0.13 | 0.03 | 0.12 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 11 | 0.13 | 0.03 | 0.12 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 11 | 0.12 | 0.02 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 11 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 11 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 11 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 11 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 11 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 11 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 11 | 0.12 | 0.02 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 11 | 0.12 | 0.02 | 0.11 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 10 | 0.14 | 0.02 | 0.14 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 10 | 0.13 | 0.02 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 10 | 0.13 | 0.02 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 10 | 0.13 | 0.02 | 0.13 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 10 | 0.11 | 0.01 | 0.11 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 9 | 0.2 | 0.03 | 0.21 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 9 | 0.15 | 0.04 | 0.15 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 9 | 0.15 | 0.04 | 0.15 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 9 | 0.15 | 0.02 | 0.15 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 9 | 0.14 | 0.04 | 0.14 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 9 | 0.14 | 0.04 | 0.14 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 9 | 0.14 | 0.04 | 0.14 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 9 | 0.14 | 0.02 | 0.14 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 9 | 0.14 | 0.02 | 0.14 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 9 | 0.12 | 0.01 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 9 | 0.12 | 0.02 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 9 | 0.12 | 0.02 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 9 | 0.12 | 0.02 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 9 | 0.12 | 0.01 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 9 | 0.12 | 0.01 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 9 | 0.12 | 0.01 | 0.12 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 8 | 0.15 | 0.06 | 0.13 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 8 | 0.15 | 0.02 | 0.15 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 8 | 0.15 | 0.02 | 0.15 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 8 | 0.11 | 0.01 | 0.11 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 8 | 0.11 | 0.01 | 0.11 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 8 | 0.11 | 0.01 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 7 | 0.2 | 0.02 | 0.21 |
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 7 | 0.2 | 0.02 | 0.21 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 7 | 0.2 | 0.02 | 0.21 |
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 7 | 0.16 | 0.02 | 0.15 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 7 | 0.13 | 0.02 | 0.13 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 7 | 0.13 | 0.02 | 0.13 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 7 | 0.13 | 0.02 | 0.13 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 7 | 0.12 | 0.01 | 0.13 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 7 | 0.12 | 0.02 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 7 | 0.12 | 0.02 | 0.12 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 7 | 0.12 | 0.01 | 0.11 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE1 | 6 | 0.18 | 0.05 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE2 | 6 | 0.18 | 0.05 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE1 | 6 | 0.18 | 0.05 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE2 | 6 | 0.18 | 0.05 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE1 | 6 | 0.18 | 0.05 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE2 | 6 | 0.18 | 0.05 | 0.16 |
| (1,1084) | 1:58:A:GLU:H | 1:118:A:LEU:HB3 | 6 | 0.14 | 0.01 | 0.15 |
| (1,1191) | 1:46:A:LYS:HB2 | 1:104:A:GLY:H | 6 | 0.13 | 0.02 | 0.12 |
| (1,718) | 1:123:A:ARG:HA | 1:126:A:GLN:HG2 | 6 | 0.12 | 0.02 | 0.11 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG11 | 6 | 0.12 | 0.01 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG12 | 6 | 0.12 | 0.01 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG13 | 6 | 0.12 | 0.01 | 0.12 |
| (1,1414) | 1:60:A:HIS:HE1 | 1:92:A:VAL:HB | 6 | 0.11 | 0.01 | 0.11 |
| (1,493) | 1:83:A:GLU:HG2 | 1:84:A:ASN:H | 6 | 0.1 | 0.0 | 0.1 |
| (1,493) | 1:83:A:GLU:HG3 | 1:84:A:ASN:H | 6 | 0.1 | 0.0 | 0.1 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG11 | 5 | 0.24 | 0.01 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG12 | 5 | 0.24 | 0.01 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG13 | 5 | 0.24 | 0.01 | 0.23 |
| (1,1204) | 1:107:A:ASN:HB2 | 1:108:A:GLY:H | 5 | 0.23 | 0.01 | 0.23 |
| (1,1512) | 1:125:A:HIS:HD2 | 1:126:A:GLN:HG3 | 5 | 0.19 | 0.05 | 0.2 |
| (1,187) | 1:33:A:ASP:HB2 | 1:34:A:ASN:H | 5 | 0.16 | 0.05 | 0.15 |
| (1,78) | 1:55:A:THR:HG21 | 1:95:A:PRO:HB2 | 5 | 0.14 | 0.04 | 0.12 |
| (1,78) | 1:55:A:THR:HG22 | 1:95:A:PRO:HB2 | 5 | 0.14 | 0.04 | 0.12 |
| (1,78) | 1:55:A:THR:HG23 | 1:95:A:PRO:HB2 | 5 | 0.14 | 0.04 | 0.12 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,217) | 1:23:A:GLY:HA3 | 1:42:A:ASN:HD22 | 5 | 0.13 | 0.01 | 0.12 |
| (1,511) | 1:80:A:GLU:HG3 | 1:87:A:TRP:HA | 5 | 0.13 | 0.01 | 0.12 |
| (1,845) | 1:74:A:LEU:HD11 | 1:103:A:GLU:HB2 | 5 | 0.12 | 0.01 | 0.12 |
| (1,845) | 1:74:A:LEU:HD12 | 1:103:A:GLU:HB2 | 5 | 0.12 | 0.01 | 0.12 |
| (1,845) | 1:74:A:LEU:HD13 | 1:103:A:GLU:HB2 | 5 | 0.12 | 0.01 | 0.12 |
| (1,1269) | 1:27:A:THR:HG21 | 1:29:A:GLY:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,1269) | 1:27:A:THR:HG22 | 1:29:A:GLY:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,1269) | 1:27:A:THR:HG23 | 1:29:A:GLY:H | 5 | 0.12 | 0.01 | 0.12 |
| (1,461) | 1:78:A:LYS:HB2 | 1:79:A:LEU:H | 5 | 0.11 | 0.01 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE1 | 5 | 0.11 | 0.01 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE2 | 5 | 0.11 | 0.01 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE3 | 5 | 0.11 | 0.01 | 0.11 |
| (1,214) | 1:22:A:VAL:HG11 | 1:23:A:GLY:H | 4 | 0.2 | 0.06 | 0.22 |
| (1,214) | 1:22:A:VAL:HG12 | 1:23:A:GLY:H | 4 | 0.2 | 0.06 | 0.22 |
| (1,214) | 1:22:A:VAL:HG13 | 1:23:A:GLY:H | 4 | 0.2 | 0.06 | 0.22 |
| (1,713) | 1:126:A:GLN:HA | 1:129:A:LYS:HG3 | 4 | 0.18 | 0.04 | 0.18 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD21 | 4 | 0.16 | 0.02 | 0.16 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD22 | 4 | 0.16 | 0.02 | 0.16 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD23 | 4 | 0.16 | 0.02 | 0.16 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD21 | 4 | 0.16 | 0.02 | 0.16 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD22 | 4 | 0.16 | 0.02 | 0.16 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD23 | 4 | 0.16 | 0.02 | 0.16 |
| (1,108) | 1:70:A:ASP:HB3 | 1:105:A:ARG:HB3 | 4 | 0.16 | 0.02 | 0.15 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD11 | 4 | 0.14 | 0.01 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD12 | 4 | 0.14 | 0.01 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD13 | 4 | 0.14 | 0.01 | 0.14 |
| (1,1356) | 1:27:A:THR:H | 1:38:A:PHE:HB2 | 4 | 0.13 | 0.01 | 0.14 |
| (1,1483) | 1:101:A:PHE:HE1 | 1:102:A:ILE:HG13 | 4 | 0.13 | 0.01 | 0.12 |
| (1,1483) | 1:101:A:PHE:HE2 | 1:102:A:ILE:HG13 | 4 | 0.13 | 0.01 | 0.12 |
| (1,265) | 1:27:A:THR:HB | 1:39:A:ARG:HB2 | 4 | 0.12 | 0.02 | 0.12 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG21 | 4 | 0.12 | 0.01 | 0.12 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG22 | 4 | 0.12 | 0.01 | 0.12 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG23 | 4 | 0.12 | 0.01 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB1 | 4 | 0.12 | 0.01 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB2 | 4 | 0.12 | 0.01 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB3 | 4 | 0.12 | 0.01 | 0.12 |
| (1,233) | 1:27:A:THR:HG21 | 1:28:A:LYS:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,233) | 1:27:A:THR:HG22 | 1:28:A:LYS:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,233) | 1:27:A:THR:HG23 | 1:28:A:LYS:H | 4 | 0.12 | 0.02 | 0.12 |
| (1,1037) | 1:24:A:GLU:H | 1:40:A:ILE:HA | 4 | 0.12 | 0.01 | 0.12 |
| (1,812) | 1:62:A:LEU:HB3 | 1:90:A:SER:HA | 4 | 0.11 | 0.01 | 0.11 |
| (1,205) | 1:15:A:VAL:HG11 | 1:16:A:ASN:H | 4 | 0.11 | 0.0 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,205) | 1:15:A:VAL:HG12 | 1:16:A:ASN:H | 4 | 0.11 | 0.0 | 0.11 |
| (1,205) | 1:15:A:VAL:HG13 | 1:16:A:ASN:H | 4 | 0.11 | 0.0 | 0.11 |
| (1,90) | 1:19:A:PRO:HA | 1:51:A:TYR:HB2 | 4 | 0.11 | 0.01 | 0.11 |
| (1,19) | 1:116:A:LEU:HD11 | 1:117:A:PRO:HD3 | 4 | 0.1 | 0.0 | 0.1 |
| (1,19) | 1:116:A:LEU:HD12 | 1:117:A:PRO:HD3 | 4 | 0.1 | 0.0 | 0.1 |
| (1,19) | 1:116:A:LEU:HD13 | 1:117:A:PRO:HD3 | 4 | 0.1 | 0.0 | 0.1 |
| (1,799) | 1:119:A:SER:HB3 | 1:120:A:GLU:HG3 | 3 | 0.22 | 0.02 | 0.21 |
| (1,1050) | 1:128:A:GLU:HB3 | 1:129:A:LYS:H | 3 | 0.2 | 0.01 | 0.19 |
| (1,841) | 1:37:A:LEU:HD11 | 1:59:A:MET:H | 3 | 0.14 | 0.02 | 0.14 |
| (1,841) | 1:37:A:LEU:HD12 | 1:59:A:MET:H | 3 | 0.14 | 0.02 | 0.14 |
| (1,841) | 1:37:A:LEU:HD13 | 1:59:A:MET:H | 3 | 0.14 | 0.02 | 0.14 |
| (1,1241) | 1:55:A:THR:H | 1:95:A:PRO:HB2 | 3 | 0.14 | 0.03 | 0.13 |
| (1,523) | 1:90:A:SER:HB3 | 1:91:A:VAL:H | 3 | 0.13 | 0.03 | 0.11 |
| (1,828) | 1:28:A:LYS:HB2 | 1:35:A:GLY:HA3 | 3 | 0.13 | 0.01 | 0.13 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG21 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG22 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG23 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG21 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG22 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG23 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG21 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG22 | 3 | 0.13 | 0.02 | 0.12 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG23 | 3 | 0.13 | 0.02 | 0.12 |
| (1,1387) | 1:14:A:TYR:HD1 | 1:18:A:ARG:HD3 | 3 | 0.13 | 0.01 | 0.12 |
| (1,1387) | 1:14:A:TYR:HD2 | 1:18:A:ARG:HD3 | 3 | 0.13 | 0.01 | 0.12 |
| (1,185) | 1:11:A:SER:HA | 1:12:A:VAL:H | 3 | 0.12 | 0.01 | 0.12 |
| (1,1211) | 1:28:A:LYS:HB2 | 1:35:A:GLY:H | 3 | 0.12 | 0.0 | 0.12 |
| (1,859) | 1:55:A:THR:H | 1:56:A:GLN:HB3 | 3 | 0.12 | 0.01 | 0.12 |
| (1,764) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HB3 | 3 | 0.11 | 0.01 | 0.11 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD1 | 3 | 0.11 | 0.01 | 0.11 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD2 | 3 | 0.11 | 0.01 | 0.11 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD21 | 3 | 0.11 | 0.01 | 0.11 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD22 | 3 | 0.11 | 0.01 | 0.11 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD23 | 3 | 0.11 | 0.01 | 0.11 |
| (1,1530) | 1:46:A:LYS:HD3 | 1:48:A:TRP:HD1 | 2 | 0.16 | 0.02 | 0.16 |
| (1,244) | 1:29:A:GLY:HA2 | 1:113:A:MET:HB2 | 2 | 0.15 | 0.03 | 0.15 |
| (1,945) | 1:74:A:LEU:H | 1:77:A:THR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (1,1513) | 1:94:A:TYR:HB3 | 1:125:A:HIS:HE1 | 2 | 0.12 | 0.0 | 0.12 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD21 | 2 | 0.12 | 0.02 | 0.12 |

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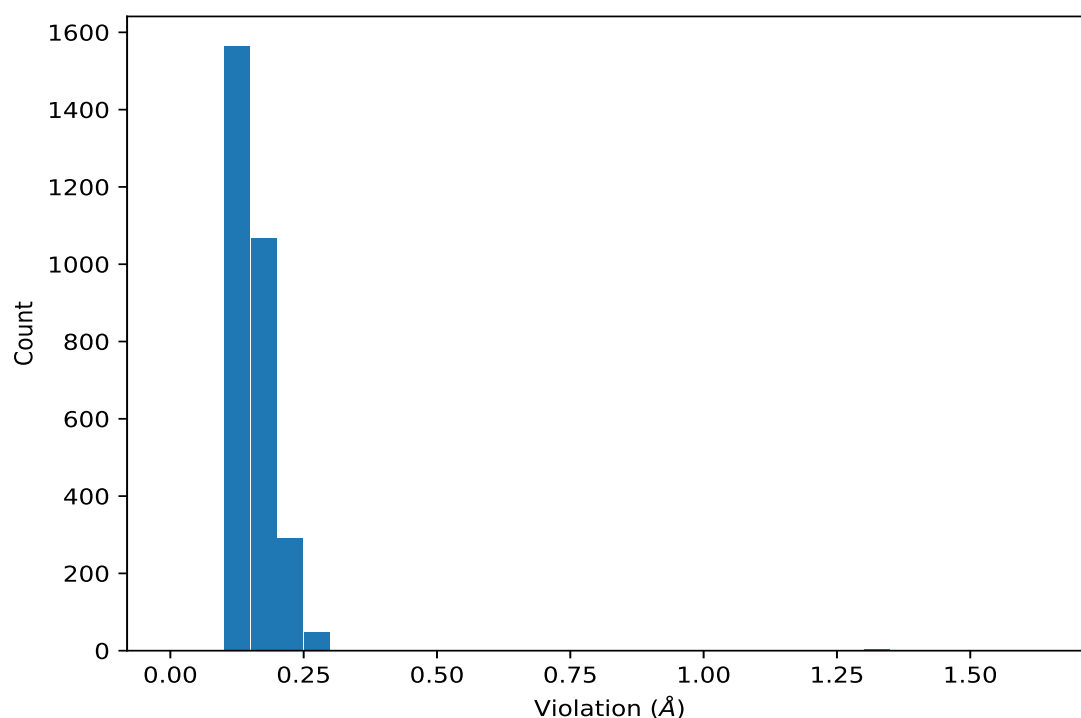
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD22 | 2 | 0.12 | 0.02 | 0.12 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD23 | 2 | 0.12 | 0.02 | 0.12 |
| (1,271) | 1:40:A:ILE:HD11 | 1:51:A:TYR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,271) | 1:40:A:ILE:HD12 | 1:51:A:TYR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,271) | 1:40:A:ILE:HD13 | 1:51:A:TYR:H | 2 | 0.12 | 0.02 | 0.12 |
| (1,924) | 1:42:A:ASN:H | 1:47:A:GLN:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (1,760) | 1:12:A:VAL:HG11 | 1:13:A:THR:HB | 2 | 0.11 | 0.0 | 0.11 |
| (1,760) | 1:12:A:VAL:HG12 | 1:13:A:THR:HB | 2 | 0.11 | 0.0 | 0.11 |
| (1,760) | 1:12:A:VAL:HG13 | 1:13:A:THR:HB | 2 | 0.11 | 0.0 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD21 | 2 | 0.11 | 0.0 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD22 | 2 | 0.11 | 0.0 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD23 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 2 | 0.11 | 0.0 | 0.11 |
| (1,1266) | 1:74:A:LEU:HD21 | 1:104:A:GLY:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,1266) | 1:74:A:LEU:HD22 | 1:104:A:GLY:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,1266) | 1:74:A:LEU:HD23 | 1:104:A:GLY:H | 2 | 0.11 | 0.01 | 0.11 |
| (1,1504) | 1:51:A:TYR:HE1 | 1:53:A:ASP:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1504) | 1:51:A:TYR:HE2 | 1:53:A:ASP:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (1,1533) | 1:46:A:LYS:HE3 | 1:48:A:TRP:HD1 | 2 | 0.1 | 0.0 | 0.1 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 1 | 1.61 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 4 | 1.57 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 2 | 1.52 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 24 | 1.51 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 7 | 1.46 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 23 | 1.43 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 22 | 1.37 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 15 | 1.35 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 6 | 1.33 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 10 | 1.33 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 17 | 1.32 |
| (1,1583) | 1:30:A:PHE:HD1 | 1:114:A:ASP:HA | 21 | 1.32 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 6 | 0.27 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 7 | 0.27 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 24 | 0.27 |
| (1,1512) | 1:125:A:HIS:HD2 | 1:126:A:GLN:HG3 | 3 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 8 | 0.26 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 8 | 0.26 |
| (1,1204) | 1:107:A:ASN:HB2 | 1:108:A:GLY:H | 11 | 0.26 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 24 | 0.26 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 24 | 0.26 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 24 | 0.26 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 10 | 0.26 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 22 | 0.26 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG11 | 19 | 0.26 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG12 | 19 | 0.26 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG13 | 19 | 0.26 |
| (1,187) | 1:33:A:ASP:HB2 | 1:34:A:ASN:H | 4 | 0.26 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 14 | 0.26 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE1 | 9 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE2 | 9 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE1 | 9 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE2 | 9 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE1 | 9 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE2 | 9 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE1 | 18 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE2 | 18 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE1 | 18 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE2 | 18 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE1 | 18 | 0.25 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE2 | 18 | 0.25 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 19 | 0.25 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 20 | 0.25 |
| (1,799) | 1:119:A:SER:HB3 | 1:120:A:GLU:HG3 | 6 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 4 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 4 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 4 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 10 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 10 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 10 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 18 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 18 | 0.25 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 18 | 0.25 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 21 | 0.25 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 10 | 0.25 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 10 | 0.25 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 10 | 0.25 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 21 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 21 | 0.25 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 21 | 0.25 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 16 | 0.25 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 20 | 0.24 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 20 | 0.24 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 20 | 0.24 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 20 | 0.24 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 20 | 0.24 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 20 | 0.24 |
| (1,1204) | 1:107:A:ASN:HB2 | 1:108:A:GLY:H | 24 | 0.24 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 12 | 0.24 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 12 | 0.24 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 12 | 0.24 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 12 | 0.24 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 14 | 0.24 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 16 | 0.24 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG11 | 4 | 0.24 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG12 | 4 | 0.24 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG13 | 4 | 0.24 |
| (1,713) | 1:126:A:GLN:HA | 1:129:A:LYS:HG3 | 6 | 0.24 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 23 | 0.24 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 16 | 0.24 |
| (1,214) | 1:22:A:VAL:HG11 | 1:23:A:GLY:H | 19 | 0.24 |
| (1,214) | 1:22:A:VAL:HG12 | 1:23:A:GLY:H | 19 | 0.24 |
| (1,214) | 1:22:A:VAL:HG13 | 1:23:A:GLY:H | 19 | 0.24 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 11 | 0.24 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 11 | 0.24 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 11 | 0.24 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 9 | 0.24 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 9 | 0.24 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 9 | 0.24 |
| (1,71) | 1:74:A:LEU:HD21 | 1:100:A:MET:HB3 | 21 | 0.24 |
| (1,71) | 1:74:A:LEU:HD22 | 1:100:A:MET:HB3 | 21 | 0.24 |
| (1,71) | 1:74:A:LEU:HD23 | 1:100:A:MET:HB3 | 21 | 0.24 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 14 | 0.23 |
| (1,1204) | 1:107:A:ASN:HB2 | 1:108:A:GLY:H | 7 | 0.23 |
| (1,1187) | 1:45:A:LYS:HB2 | 1:47:A:GLN:H | 3 | 0.23 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 1 | 0.23 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 1 | 0.23 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 1 | 0.23 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 16 | 0.23 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 16 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 16 | 0.23 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 2 | 0.23 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 1 | 0.23 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 5 | 0.23 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 11 | 0.23 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 11 | 0.23 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 11 | 0.23 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 17 | 0.23 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 22 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG11 | 2 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG12 | 2 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG13 | 2 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG11 | 22 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG12 | 22 | 0.23 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG13 | 22 | 0.23 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 2 | 0.23 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 9 | 0.23 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 10 | 0.23 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 1 | 0.23 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 1 | 0.23 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 1 | 0.23 |
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 15 | 0.23 |
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 15 | 0.23 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 15 | 0.23 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 2 | 0.23 |
| (1,214) | 1:22:A:VAL:HG11 | 1:23:A:GLY:H | 5 | 0.23 |
| (1,214) | 1:22:A:VAL:HG12 | 1:23:A:GLY:H | 5 | 0.23 |
| (1,214) | 1:22:A:VAL:HG13 | 1:23:A:GLY:H | 5 | 0.23 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 18 | 0.23 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 18 | 0.23 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 18 | 0.23 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 4 | 0.23 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 7 | 0.23 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 7 | 0.23 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 7 | 0.23 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 19 | 0.23 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 19 | 0.23 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 19 | 0.23 |
| (1,1664) | 1:71:A:ILE:HG21 | 1:87:A:TRP:HD1 | 19 | 0.22 |
| (1,1664) | 1:71:A:ILE:HG22 | 1:87:A:TRP:HD1 | 19 | 0.22 |
| (1,1664) | 1:71:A:ILE:HG23 | 1:87:A:TRP:HD1 | 19 | 0.22 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 13 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 13 | 0.22 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 7 | 0.22 |
| (1,1204) | 1:107:A:ASN:HB2 | 1:108:A:GLY:H | 1 | 0.22 |
| (1,1204) | 1:107:A:ASN:HB2 | 1:108:A:GLY:H | 12 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 6 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 6 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 6 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 11 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 11 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 11 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 17 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 17 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 17 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 22 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 22 | 0.22 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 22 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 2 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 2 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 2 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 7 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 7 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 7 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 19 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 19 | 0.22 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 19 | 0.22 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 4 | 0.22 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 17 | 0.22 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 19 | 0.22 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 20 | 0.22 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG11 | 16 | 0.22 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG12 | 16 | 0.22 |
| (1,745) | 1:11:A:SER:HA | 1:12:A:VAL:HG13 | 16 | 0.22 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 11 | 0.22 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 13 | 0.22 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 15 | 0.22 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 3 | 0.22 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 3 | 0.22 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 3 | 0.22 |
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 1 | 0.22 |
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 1 | 0.22 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 1 | 0.22 |
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 11 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 11 | 0.22 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 11 | 0.22 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 17 | 0.22 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 17 | 0.22 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 17 | 0.22 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 7 | 0.22 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 24 | 0.22 |
| (1,214) | 1:22:A:VAL:HG11 | 1:23:A:GLY:H | 23 | 0.22 |
| (1,214) | 1:22:A:VAL:HG12 | 1:23:A:GLY:H | 23 | 0.22 |
| (1,214) | 1:22:A:VAL:HG13 | 1:23:A:GLY:H | 23 | 0.22 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 15 | 0.22 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 15 | 0.22 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 15 | 0.22 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 23 | 0.22 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 23 | 0.22 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 23 | 0.22 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 17 | 0.22 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 24 | 0.21 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 24 | 0.21 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 24 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 8 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 8 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 8 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 8 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 8 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 8 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 17 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 17 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 17 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 17 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 17 | 0.21 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 17 | 0.21 |
| (1,1512) | 1:125:A:HIS:HD2 | 1:126:A:GLN:HG3 | 14 | 0.21 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 16 | 0.21 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 16 | 0.21 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 16 | 0.21 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 16 | 0.21 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 16 | 0.21 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 16 | 0.21 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 22 | 0.21 |
| (1,1050) | 1:128:A:GLU:HB3 | 1:129:A:LYS:H | 15 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 6 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 6 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 6 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 8 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 8 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 8 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 14 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 14 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 14 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 20 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 20 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 20 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 24 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 24 | 0.21 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 24 | 0.21 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 20 | 0.21 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 10 | 0.21 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 11 | 0.21 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 23 | 0.21 |
| (1,799) | 1:119:A:SER:HB3 | 1:120:A:GLU:HG3 | 4 | 0.21 |
| (1,799) | 1:119:A:SER:HB3 | 1:120:A:GLU:HG3 | 12 | 0.21 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 4 | 0.21 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 7 | 0.21 |
| (1,713) | 1:126:A:GLN:HA | 1:129:A:LYS:HG3 | 21 | 0.21 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 4 | 0.21 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 8 | 0.21 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 14 | 0.21 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 24 | 0.21 |
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 19 | 0.21 |
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 19 | 0.21 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 19 | 0.21 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 15 | 0.21 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 16 | 0.21 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 19 | 0.21 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 1 | 0.21 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 1 | 0.21 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 1 | 0.21 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 14 | 0.21 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 14 | 0.21 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 14 | 0.21 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 20 | 0.21 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 20 | 0.21 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 20 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 16 | 0.21 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 16 | 0.21 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 16 | 0.21 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 9 | 0.2 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 9 | 0.2 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 9 | 0.2 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 10 | 0.2 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 10 | 0.2 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 10 | 0.2 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 2 | 0.2 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 2 | 0.2 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 2 | 0.2 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 6 | 0.2 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 6 | 0.2 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 6 | 0.2 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 14 | 0.2 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 14 | 0.2 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 14 | 0.2 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 14 | 0.2 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 14 | 0.2 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 14 | 0.2 |
| (1,1512) | 1:125:A:HIS:HD2 | 1:126:A:GLN:HG3 | 22 | 0.2 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 8 | 0.2 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 8 | 0.2 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 8 | 0.2 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 8 | 0.2 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 8 | 0.2 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 8 | 0.2 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 1 | 0.2 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 1 | 0.2 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 1 | 0.2 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 1 | 0.2 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 1 | 0.2 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 1 | 0.2 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 6 | 0.2 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 6 | 0.2 |
| (1,1352) | 1:54:A:THR:H | 1:57:A:TYR:HD1 | 11 | 0.2 |
| (1,1352) | 1:54:A:THR:H | 1:57:A:TYR:HD2 | 11 | 0.2 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 23 | 0.2 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 24 | 0.2 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 21 | 0.2 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 21 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 21 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 11 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 11 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 11 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 12 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 12 | 0.2 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 12 | 0.2 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 11 | 0.2 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 2 | 0.2 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 7 | 0.2 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 15 | 0.2 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 15 | 0.2 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 15 | 0.2 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 15 | 0.2 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 14 | 0.2 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 3 | 0.2 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 12 | 0.2 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 16 | 0.2 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 20 | 0.2 |
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 24 | 0.2 |
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 24 | 0.2 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 24 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 3 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 5 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 8 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 10 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 11 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 12 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 13 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 20 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 21 | 0.2 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 23 | 0.2 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 3 | 0.2 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 3 | 0.2 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 3 | 0.2 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 24 | 0.2 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 24 | 0.2 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 24 | 0.2 |
| (1,171) | 1:18:A:ARG:HA | 1:19:A:PRO:HD2 | 5 | 0.2 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 13 | 0.2 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 13 | 0.2 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 13 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 19 | 0.2 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 5 | 0.19 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 5 | 0.19 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 5 | 0.19 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 12 | 0.19 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 12 | 0.19 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 12 | 0.19 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 23 | 0.19 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 23 | 0.19 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 23 | 0.19 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 19 | 0.19 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 19 | 0.19 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 19 | 0.19 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 22 | 0.19 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 22 | 0.19 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 22 | 0.19 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 13 | 0.19 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 13 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 7 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 7 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 7 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 7 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 7 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 7 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 13 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 13 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 13 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 13 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 13 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 13 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 14 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 14 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 14 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 14 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 14 | 0.19 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 14 | 0.19 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 10 | 0.19 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 10 | 0.19 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 10 | 0.19 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 20 | 0.19 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 20 | 0.19 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 20 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 20 | 0.19 |
| (1,1050) | 1:128:A:GLU:HB3 | 1:129:A:LYS:H | 3 | 0.19 |
| (1,1050) | 1:128:A:GLU:HB3 | 1:129:A:LYS:H | 21 | 0.19 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 9 | 0.19 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 9 | 0.19 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 9 | 0.19 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 15 | 0.19 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 15 | 0.19 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 15 | 0.19 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 13 | 0.19 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 16 | 0.19 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 3 | 0.19 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 12 | 0.19 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 19 | 0.19 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 21 | 0.19 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 22 | 0.19 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 13 | 0.19 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 16 | 0.19 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 16 | 0.19 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 16 | 0.19 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 22 | 0.19 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 22 | 0.19 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 22 | 0.19 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 1 | 0.19 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 4 | 0.19 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 6 | 0.19 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 9 | 0.19 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 18 | 0.19 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 7 | 0.19 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 7 | 0.19 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 7 | 0.19 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 13 | 0.19 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 13 | 0.19 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 13 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 9 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 9 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 9 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 11 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 11 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 11 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 19 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 19 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 19 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 21 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 21 | 0.19 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 21 | 0.19 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 13 | 0.19 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 13 | 0.19 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 13 | 0.19 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 13 | 0.19 |
| (1,108) | 1:70:A:ASP:HB3 | 1:105:A:ARG:HB3 | 11 | 0.19 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD21 | 15 | 0.19 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD22 | 15 | 0.19 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD23 | 15 | 0.19 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD21 | 15 | 0.19 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD22 | 15 | 0.19 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD23 | 15 | 0.19 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 10 | 0.19 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 10 | 0.19 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 10 | 0.19 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 13 | 0.19 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 13 | 0.19 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 13 | 0.19 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 20 | 0.19 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 20 | 0.19 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 20 | 0.19 |
| (1,78) | 1:55:A:THR:HG21 | 1:95:A:PRO:HB2 | 9 | 0.19 |
| (1,78) | 1:55:A:THR:HG22 | 1:95:A:PRO:HB2 | 9 | 0.19 |
| (1,78) | 1:55:A:THR:HG23 | 1:95:A:PRO:HB2 | 9 | 0.19 |
| (1,78) | 1:55:A:THR:HG21 | 1:95:A:PRO:HB2 | 18 | 0.19 |
| (1,78) | 1:55:A:THR:HG22 | 1:95:A:PRO:HB2 | 18 | 0.19 |
| (1,78) | 1:55:A:THR:HG23 | 1:95:A:PRO:HB2 | 18 | 0.19 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 13 | 0.18 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 13 | 0.18 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 13 | 0.18 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 14 | 0.18 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 14 | 0.18 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 14 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 8 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 8 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 8 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 19 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 19 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 19 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 21 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 21 | 0.18 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 21 | 0.18 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 17 | 0.18 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 17 | 0.18 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 17 | 0.18 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 22 | 0.18 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 22 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 10 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 10 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 10 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 10 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 10 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 10 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 12 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 12 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 12 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 12 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 12 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 12 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 19 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 19 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 19 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 19 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 19 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 19 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 21 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 21 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 21 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 21 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 21 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 21 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 22 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 22 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 22 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 22 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 22 | 0.18 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 22 | 0.18 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 15 | 0.18 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 15 | 0.18 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 9 | 0.18 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 9 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 19 | 0.18 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 19 | 0.18 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 12 | 0.18 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 12 | 0.18 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 12 | 0.18 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 12 | 0.18 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 12 | 0.18 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 12 | 0.18 |
| (1,1298) | 1:127:A:ALA:H | 1:128:A:GLU:HG2 | 7 | 0.18 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 9 | 0.18 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 9 | 0.18 |
| (1,1241) | 1:55:A:THR:H | 1:95:A:PRO:HB2 | 13 | 0.18 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 11 | 0.18 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 13 | 0.18 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 16 | 0.18 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 11 | 0.18 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 16 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 2 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 2 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 2 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 4 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 4 | 0.18 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 4 | 0.18 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 9 | 0.18 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 11 | 0.18 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 14 | 0.18 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 18 | 0.18 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 19 | 0.18 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 23 | 0.18 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 5 | 0.18 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 5 | 0.18 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 5 | 0.18 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 18 | 0.18 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 18 | 0.18 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 18 | 0.18 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 3 | 0.18 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 8 | 0.18 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 18 | 0.18 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 24 | 0.18 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 19 | 0.18 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 19 | 0.18 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 19 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 4 | 0.18 |
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 16 | 0.18 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 10 | 0.18 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 19 | 0.18 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 20 | 0.18 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 5 | 0.18 |
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 7 | 0.18 |
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 7 | 0.18 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 7 | 0.18 |
| (1,523) | 1:90:A:SER:HB3 | 1:91:A:VAL:H | 23 | 0.18 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 16 | 0.18 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 3 | 0.18 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 18 | 0.18 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 18 | 0.18 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 18 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 1 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 1 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 1 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 4 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 4 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 4 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 5 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 5 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 5 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 6 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 6 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 6 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 7 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 7 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 7 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 9 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 9 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 9 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 15 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 15 | 0.18 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 15 | 0.18 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 14 | 0.18 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 17 | 0.18 |
| (1,282) | 1:67:A:GLU:HG3 | 1:68:A:ASP:H | 22 | 0.18 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 6 | 0.18 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 6 | 0.18 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 6 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 16 | 0.18 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 16 | 0.18 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 16 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 2 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 2 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 2 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 6 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 6 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 6 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 8 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 8 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 8 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 10 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 10 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 10 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 15 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 15 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 15 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 20 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 20 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 20 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 23 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 23 | 0.18 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 23 | 0.18 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 2 | 0.18 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 8 | 0.18 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 9 | 0.18 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 11 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 6 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 6 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 6 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 22 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 22 | 0.18 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 22 | 0.18 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD21 | 14 | 0.18 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD22 | 14 | 0.18 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD23 | 14 | 0.18 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD21 | 14 | 0.18 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD22 | 14 | 0.18 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD23 | 14 | 0.18 |
| (1,1671) | 1:126:A:GLN:HA | 1:129:A:LYS:HB3 | 8 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 1 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 1 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 8 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 8 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 8 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 22 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 22 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 22 | 0.17 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 8 | 0.17 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 8 | 0.17 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 8 | 0.17 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 16 | 0.17 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 16 | 0.17 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 16 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 2 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 2 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 2 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 7 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 7 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 7 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 11 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 11 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 11 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 16 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 16 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 16 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 18 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 18 | 0.17 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 18 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 4 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 4 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 4 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 5 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 5 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 5 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 9 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 9 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 9 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 10 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 10 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 10 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 16 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 16 | 0.17 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 16 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 1 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 1 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 1 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 5 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 5 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 5 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 8 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 8 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 8 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 18 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 18 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 18 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 19 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 19 | 0.17 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 19 | 0.17 |
| (1,1530) | 1:46:A:LYS:HD3 | 1:48:A:TRP:HD1 | 12 | 0.17 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 2 | 0.17 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 2 | 0.17 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 2 | 0.17 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 2 | 0.17 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 2 | 0.17 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 2 | 0.17 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE1 | 23 | 0.17 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE2 | 23 | 0.17 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE1 | 23 | 0.17 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE2 | 23 | 0.17 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE1 | 23 | 0.17 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE2 | 23 | 0.17 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 11 | 0.17 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 11 | 0.17 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 24 | 0.17 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 24 | 0.17 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 4 | 0.17 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 4 | 0.17 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 4 | 0.17 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 4 | 0.17 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 4 | 0.17 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 4 | 0.17 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 12 | 0.17 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 12 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 12 | 0.17 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 18 | 0.17 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 18 | 0.17 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 18 | 0.17 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 1 | 0.17 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 12 | 0.17 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 8 | 0.17 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 8 | 0.17 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 8 | 0.17 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 3 | 0.17 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 6 | 0.17 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 8 | 0.17 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 16 | 0.17 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 24 | 0.17 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 1 | 0.17 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 1 | 0.17 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 1 | 0.17 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 21 | 0.17 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 21 | 0.17 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 21 | 0.17 |
| (1,971) | 1:64:A:THR:H | 1:110:A:LYS:HG2 | 12 | 0.17 |
| (1,971) | 1:64:A:THR:H | 1:110:A:LYS:HG3 | 12 | 0.17 |
| (1,841) | 1:37:A:LEU:HD11 | 1:59:A:MET:H | 16 | 0.17 |
| (1,841) | 1:37:A:LEU:HD12 | 1:59:A:MET:H | 16 | 0.17 |
| (1,841) | 1:37:A:LEU:HD13 | 1:59:A:MET:H | 16 | 0.17 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 1 | 0.17 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 1 | 0.17 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 1 | 0.17 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 6 | 0.17 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 9 | 0.17 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 15 | 0.17 |
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 20 | 0.17 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 12 | 0.17 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 12 | 0.17 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 1 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 24 | 0.17 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 7 | 0.17 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 17 | 0.17 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 18 | 0.17 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 11 | 0.17 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 11 | 0.17 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 11 | 0.17 |
| (1,574) | 1:100:A:MET:HE1 | 1:101:A:PHE:HA | 14 | 0.17 |
| (1,574) | 1:100:A:MET:HE2 | 1:101:A:PHE:HA | 14 | 0.17 |
| (1,574) | 1:100:A:MET:HE3 | 1:101:A:PHE:HA | 14 | 0.17 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 19 | 0.17 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 21 | 0.17 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 9 | 0.17 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 18 | 0.17 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 19 | 0.17 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 24 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 2 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 2 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 2 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 18 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 18 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 18 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 23 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 23 | 0.17 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 23 | 0.17 |
| (1,244) | 1:29:A:GLY:HA2 | 1:113:A:MET:HB2 | 17 | 0.17 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 4 | 0.17 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 4 | 0.17 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 4 | 0.17 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 5 | 0.17 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 5 | 0.17 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 5 | 0.17 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 12 | 0.17 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 12 | 0.17 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 12 | 0.17 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 14 | 0.17 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 14 | 0.17 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 14 | 0.17 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 24 | 0.17 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 24 | 0.17 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 24 | 0.17 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 22 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 2 | 0.17 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 2 | 0.17 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 2 | 0.17 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 5 | 0.17 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 5 | 0.17 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 5 | 0.17 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 19 | 0.17 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 19 | 0.17 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 19 | 0.17 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 15 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 15 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 15 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 19 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 19 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 19 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 21 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 21 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 21 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 2 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 2 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 2 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 9 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 9 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 9 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 15 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 15 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 15 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 18 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 18 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 18 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 20 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 20 | 0.16 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 20 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 1 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 1 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 1 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 3 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 3 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 3 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 5 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 5 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 5 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|---------------|-----------------|----------|---------------|
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 6 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 6 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 6 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 13 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 13 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 13 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 14 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 14 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 14 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 15 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 15 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 15 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 24 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 24 | 0.16 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 24 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 1 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 1 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 1 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 7 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 7 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 7 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 8 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 8 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 8 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 13 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 13 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 13 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 23 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 23 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 23 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 24 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 24 | 0.16 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 24 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 2 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 2 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 2 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 3 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 3 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 3 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 4 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 4 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 6 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 6 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 6 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 7 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 7 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 7 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 10 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 10 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 10 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 15 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 15 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 15 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 16 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 16 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 16 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 17 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 17 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 17 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 23 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 23 | 0.16 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 23 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 3 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 3 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 3 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 3 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 3 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 3 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 4 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 4 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 4 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 4 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 4 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 4 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 6 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 6 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 6 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 6 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 6 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 6 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 15 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 15 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 15 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 15 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 15 | 0.16 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 15 | 0.16 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 17 | 0.16 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 17 | 0.16 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 20 | 0.16 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 20 | 0.16 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 21 | 0.16 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 21 | 0.16 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 4 | 0.16 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 4 | 0.16 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 14 | 0.16 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 14 | 0.16 |
| (1,1512) | 1:125:A:HIS:HD2 | 1:126:A:GLN:HG3 | 16 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE1 | 1 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE2 | 1 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE1 | 1 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE2 | 1 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE1 | 1 | 0.16 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE2 | 1 | 0.16 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 14 | 0.16 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 14 | 0.16 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 5 | 0.16 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 5 | 0.16 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 5 | 0.16 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 6 | 0.16 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 6 | 0.16 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 18 | 0.16 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 7 | 0.16 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 24 | 0.16 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 10 | 0.16 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 1 | 0.16 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 7 | 0.16 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 14 | 0.16 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 14 | 0.16 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 14 | 0.16 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 19 | 0.16 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 19 | 0.16 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 19 | 0.16 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 13 | 0.16 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 15 | 0.16 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 17 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 21 | 0.16 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 3 | 0.16 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 3 | 0.16 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 3 | 0.16 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 10 | 0.16 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 10 | 0.16 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 10 | 0.16 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 17 | 0.16 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 9 | 0.16 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 9 | 0.16 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 9 | 0.16 |
| (1,858) | 1:54:A:THR:HB | 1:55:A:THR:H | 8 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 10 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 10 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 10 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 14 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 14 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 14 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 24 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 24 | 0.16 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 24 | 0.16 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 12 | 0.16 |
| (1,718) | 1:123:A:ARG:HA | 1:126:A:GLN:HG2 | 20 | 0.16 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 13 | 0.16 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 19 | 0.16 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 19 | 0.16 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 11 | 0.16 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 17 | 0.16 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 20 | 0.16 |
| (1,598) | 1:47:A:GLN:HG2 | 1:103:A:GLU:HA | 1 | 0.16 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG21 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG22 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG23 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG21 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG22 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG23 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG21 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG22 | 19 | 0.16 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG23 | 19 | 0.16 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 7 | 0.16 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 8 | 0.16 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 15 | 0.16 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 4 | 0.16 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 5 | 0.16 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 14 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 3 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 3 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 3 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 12 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 12 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 12 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 13 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 13 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 13 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 24 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 24 | 0.16 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 24 | 0.16 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 17 | 0.16 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 17 | 0.16 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 17 | 0.16 |
| (1,187) | 1:33:A:ASP:HB2 | 1:34:A:ASN:H | 22 | 0.16 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 7 | 0.16 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 7 | 0.16 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 7 | 0.16 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 23 | 0.16 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 3 | 0.16 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 23 | 0.16 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 23 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 23 | 0.16 |
| (1,108) | 1:70:A:ASP:HB3 | 1:105:A:ARG:HB3 | 4 | 0.16 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 6 | 0.15 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 6 | 0.15 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 6 | 0.15 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 18 | 0.15 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 18 | 0.15 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 18 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 13 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 13 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 13 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 17 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 17 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 17 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 22 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 22 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 22 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 23 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 23 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 23 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 4 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 4 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 4 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 12 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 12 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 12 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 17 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 17 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 17 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 22 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 22 | 0.15 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 22 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 3 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 3 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 3 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 11 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 11 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 11 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 14 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 14 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 14 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 15 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 15 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 15 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 20 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 20 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 20 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 21 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 21 | 0.15 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 21 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 9 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 9 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 9 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 11 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 11 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 11 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 12 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 12 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 12 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 13 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 13 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 13 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 14 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 14 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 14 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 22 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 22 | 0.15 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 22 | 0.15 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 2 | 0.15 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 2 | 0.15 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 16 | 0.15 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 16 | 0.15 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 19 | 0.15 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 19 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 1 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 1 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 1 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 1 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 1 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 1 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 16 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 16 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 16 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 16 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 16 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 16 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 23 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 23 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 23 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 23 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 23 | 0.15 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 23 | 0.15 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 2 | 0.15 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 2 | 0.15 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 17 | 0.15 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 17 | 0.15 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE1 | 19 | 0.15 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE2 | 19 | 0.15 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE1 | 19 | 0.15 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE2 | 19 | 0.15 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE1 | 19 | 0.15 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE2 | 19 | 0.15 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 20 | 0.15 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 20 | 0.15 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 23 | 0.15 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 23 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 2 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 2 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 2 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 2 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 2 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 2 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 9 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 9 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 9 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 9 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 9 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 9 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 17 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 17 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 17 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 17 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 17 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 17 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 22 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 22 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 22 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 22 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 22 | 0.15 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 22 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 17 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 17 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 17 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 17 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 17 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 17 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 18 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 18 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 18 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 18 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 18 | 0.15 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 18 | 0.15 |
| (1,1356) | 1:27:A:THR:H | 1:38:A:PHE:HB2 | 21 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 1 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 1 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 1 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 10 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 10 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 10 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 15 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 15 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 15 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 21 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 21 | 0.15 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 21 | 0.15 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 16 | 0.15 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 16 | 0.15 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 8 | 0.15 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 8 | 0.15 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 4 | 0.15 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 8 | 0.15 |
| (1,1191) | 1:46:A:LYS:HB2 | 1:104:A:GLY:H | 7 | 0.15 |
| (1,1191) | 1:46:A:LYS:HB2 | 1:104:A:GLY:H | 16 | 0.15 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 4 | 0.15 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 5 | 0.15 |
| (1,1146) | 1:99:A:GLU:HB2 | 1:50:A:TYR:H | 5 | 0.15 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 21 | 0.15 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 18 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 1 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 3 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 7 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 8 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 9 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 10 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 12 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 14 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 15 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 18 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 20 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 22 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 23 | 0.15 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 24 | 0.15 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 9 | 0.15 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 9 | 0.15 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 9 | 0.15 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 16 | 0.15 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 16 | 0.15 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 16 | 0.15 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 1 | 0.15 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 2 | 0.15 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 7 | 0.15 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 10 | 0.15 |
| (1,1084) | 1:58:A:GLU:H | 1:118:A:LEU:HB3 | 12 | 0.15 |
| (1,1084) | 1:58:A:GLU:H | 1:118:A:LEU:HB3 | 20 | 0.15 |
| (1,1084) | 1:58:A:GLU:H | 1:118:A:LEU:HB3 | 22 | 0.15 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 7 | 0.15 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 8 | 0.15 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 16 | 0.15 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 24 | 0.15 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 24 | 0.15 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 24 | 0.15 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 6 | 0.15 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 21 | 0.15 |
| (1,828) | 1:28:A:LYS:HB2 | 1:35:A:GLY:HA3 | 18 | 0.15 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 8 | 0.15 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 8 | 0.15 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 8 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 7 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 7 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 7 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 18 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 18 | 0.15 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 18 | 0.15 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 9 | 0.15 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 1 | 0.15 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 2 | 0.15 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 21 | 0.15 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 24 | 0.15 |
| (1,713) | 1:126:A:GLN:HA | 1:129:A:LYS:HG3 | 15 | 0.15 |
| (1,698) | 1:121:A:GLU:HG3 | 1:122:A:TYR:H | 22 | 0.15 |
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 17 | 0.15 |
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 22 | 0.15 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 22 | 0.15 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 6 | 0.15 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 6 | 0.15 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 6 | 0.15 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 12 | 0.15 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 12 | 0.15 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 12 | 0.15 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 17 | 0.15 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 17 | 0.15 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 17 | 0.15 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 24 | 0.15 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 24 | 0.15 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 24 | 0.15 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 5 | 0.15 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 13 | 0.15 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 14 | 0.15 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 22 | 0.15 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 19 | 0.15 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 21 | 0.15 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 21 | 0.15 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 8 | 0.15 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 8 | 0.15 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 8 | 0.15 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 18 | 0.15 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 20 | 0.15 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 3 | 0.15 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 11 | 0.15 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 14 | 0.15 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 16 | 0.15 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 21 | 0.15 |
| (1,511) | 1:80:A:GLU:HG3 | 1:87:A:TRP:HA | 16 | 0.15 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 12 | 0.15 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 17 | 0.15 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 2 | 0.15 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 2 | 0.15 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 2 | 0.15 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 1 | 0.15 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 1 | 0.15 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 1 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 8 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 8 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 8 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 11 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 11 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 11 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 19 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 19 | 0.15 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,265) | 1:27:A:THR:HB | 1:39:A:ARG:HB2 | 24 | 0.15 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 8 | 0.15 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 8 | 0.15 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 8 | 0.15 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 19 | 0.15 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 19 | 0.15 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 19 | 0.15 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 22 | 0.15 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 22 | 0.15 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 22 | 0.15 |
| (1,187) | 1:33:A:ASP:HB2 | 1:34:A:ASN:H | 6 | 0.15 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 4 | 0.15 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 4 | 0.15 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 4 | 0.15 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 16 | 0.15 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 16 | 0.15 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 16 | 0.15 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 21 | 0.15 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 4 | 0.15 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 4 | 0.15 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 4 | 0.15 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 12 | 0.15 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 12 | 0.15 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 12 | 0.15 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 5 | 0.15 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 5 | 0.15 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 5 | 0.15 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 5 | 0.15 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 7 | 0.15 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 7 | 0.15 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 7 | 0.15 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD21 | 7 | 0.15 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD22 | 7 | 0.15 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD23 | 7 | 0.15 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD21 | 7 | 0.15 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD22 | 7 | 0.15 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD23 | 7 | 0.15 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 11 | 0.15 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 11 | 0.15 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 11 | 0.15 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD11 | 22 | 0.15 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD12 | 22 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD13 | 22 | 0.15 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 1 | 0.15 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 18 | 0.15 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 18 | 0.15 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 4 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 4 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 4 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 5 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 5 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 5 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 6 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 6 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 6 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 10 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 10 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 10 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 19 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 19 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 19 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 21 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 21 | 0.14 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 21 | 0.14 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 9 | 0.14 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 9 | 0.14 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 9 | 0.14 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG11 | 20 | 0.14 |
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG12 | 20 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1614) | 1:61:A:VAL:H | 1:61:A:VAL:HG13 | 20 | 0.14 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 12 | 0.14 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 12 | 0.14 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 12 | 0.14 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG21 | 18 | 0.14 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG22 | 18 | 0.14 |
| (1,1609) | 1:15:A:VAL:H | 1:15:A:VAL:HG23 | 18 | 0.14 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 20 | 0.14 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 20 | 0.14 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 20 | 0.14 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 24 | 0.14 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 24 | 0.14 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 24 | 0.14 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 9 | 0.14 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 9 | 0.14 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 17 | 0.14 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 17 | 0.14 |
| (1,1530) | 1:46:A:LYS:HD3 | 1:48:A:TRP:HD1 | 22 | 0.14 |
| (1,1521) | 1:122:A:TYR:HD1 | 1:123:A:ARG:HA | 10 | 0.14 |
| (1,1521) | 1:122:A:TYR:HD2 | 1:123:A:ARG:HA | 10 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 11 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 11 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 11 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 11 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 11 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 11 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 13 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 13 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 13 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 13 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 13 | 0.14 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 13 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 3 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 3 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 16 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 16 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 20 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 20 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 23 | 0.14 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 23 | 0.14 |
| (1,1505) | 1:92:A:VAL:HG11 | 1:94:A:TYR:HE1 | 8 | 0.14 |
| (1,1505) | 1:92:A:VAL:HG11 | 1:94:A:TYR:HE2 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1505) | 1:92:A:VAL:HG12 | 1:94:A:TYR:HE1 | 8 | 0.14 |
| (1,1505) | 1:92:A:VAL:HG12 | 1:94:A:TYR:HE2 | 8 | 0.14 |
| (1,1505) | 1:92:A:VAL:HG13 | 1:94:A:TYR:HE1 | 8 | 0.14 |
| (1,1505) | 1:92:A:VAL:HG13 | 1:94:A:TYR:HE2 | 8 | 0.14 |
| (1,1483) | 1:101:A:PHE:HE1 | 1:102:A:ILE:HG13 | 4 | 0.14 |
| (1,1483) | 1:101:A:PHE:HE2 | 1:102:A:ILE:HG13 | 4 | 0.14 |
| (1,1387) | 1:14:A:TYR:HD1 | 1:18:A:ARG:HD3 | 6 | 0.14 |
| (1,1387) | 1:14:A:TYR:HD2 | 1:18:A:ARG:HD3 | 6 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 6 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 6 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 6 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 6 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 6 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 6 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 15 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 15 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 15 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 15 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 15 | 0.14 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 15 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 6 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 6 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 6 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 6 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 6 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 6 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 7 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 7 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 7 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 7 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 7 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 7 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 10 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 10 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 10 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 10 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 10 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 10 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 13 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 13 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 13 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 13 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 13 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 13 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 19 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 19 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 19 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 19 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 19 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 19 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 23 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 23 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 23 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 23 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 23 | 0.14 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 23 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 8 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 8 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 12 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 12 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 16 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 16 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 23 | 0.14 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 23 | 0.14 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG11 | 1 | 0.14 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG12 | 1 | 0.14 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG13 | 1 | 0.14 |
| (1,1356) | 1:27:A:THR:H | 1:38:A:PHE:HB2 | 10 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 2 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 2 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 2 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 3 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 3 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 3 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 6 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 6 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 6 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 9 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 9 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 9 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 17 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 17 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 17 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 20 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 20 | 0.14 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 20 | 0.14 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 4 | 0.14 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 4 | 0.14 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 18 | 0.14 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 18 | 0.14 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 3 | 0.14 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 13 | 0.14 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 13 | 0.14 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 18 | 0.14 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 24 | 0.14 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 3 | 0.14 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 11 | 0.14 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 17 | 0.14 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 21 | 0.14 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 22 | 0.14 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 2 | 0.14 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 6 | 0.14 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 13 | 0.14 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 16 | 0.14 |
| (1,1130) | 1:70:A:ASP:HB3 | 1:71:A:ILE:H | 21 | 0.14 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 15 | 0.14 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 15 | 0.14 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 15 | 0.14 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 23 | 0.14 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 23 | 0.14 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 23 | 0.14 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 4 | 0.14 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 12 | 0.14 |
| (1,1084) | 1:58:A:GLU:H | 1:118:A:LEU:HB3 | 4 | 0.14 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG11 | 23 | 0.14 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG12 | 23 | 0.14 |
| (1,1025) | 1:21:A:PHE:H | 1:22:A:VAL:HG13 | 23 | 0.14 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 6 | 0.14 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 13 | 0.14 |
| (1,945) | 1:74:A:LEU:H | 1:77:A:THR:H | 14 | 0.14 |
| (1,841) | 1:37:A:LEU:HD11 | 1:59:A:MET:H | 10 | 0.14 |
| (1,841) | 1:37:A:LEU:HD12 | 1:59:A:MET:H | 10 | 0.14 |
| (1,841) | 1:37:A:LEU:HD13 | 1:59:A:MET:H | 10 | 0.14 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG21 | 9 | 0.14 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG22 | 9 | 0.14 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG23 | 9 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 5 | 0.14 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 5 | 0.14 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 5 | 0.14 |
| (1,757) | 1:94:A:TYR:HB2 | 1:95:A:PRO:HD3 | 18 | 0.14 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 8 | 0.14 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 18 | 0.14 |
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 14 | 0.14 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 24 | 0.14 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 24 | 0.14 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 21 | 0.14 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 21 | 0.14 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 21 | 0.14 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 2 | 0.14 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 7 | 0.14 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 15 | 0.14 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 18 | 0.14 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 21 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 2 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 3 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 8 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 9 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 14 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 15 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 18 | 0.14 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 19 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 4 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 5 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 6 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 10 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 13 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 20 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 22 | 0.14 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 24 | 0.14 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 11 | 0.14 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 1 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 18 | 0.14 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 17 | 0.14 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 17 | 0.14 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 17 | 0.14 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 3 | 0.14 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 3 | 0.14 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 3 | 0.14 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 7 | 0.14 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 7 | 0.14 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 7 | 0.14 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 12 | 0.14 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 12 | 0.14 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 12 | 0.14 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 16 | 0.14 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 16 | 0.14 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 16 | 0.14 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 19 | 0.14 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 19 | 0.14 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 19 | 0.14 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 21 | 0.14 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 21 | 0.14 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 21 | 0.14 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB1 | 19 | 0.14 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB2 | 19 | 0.14 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB3 | 19 | 0.14 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 1 | 0.14 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 5 | 0.14 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 19 | 0.14 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 10 | 0.14 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 10 | 0.14 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 10 | 0.14 |
| (1,233) | 1:27:A:THR:HG21 | 1:28:A:LYS:H | 18 | 0.14 |
| (1,233) | 1:27:A:THR:HG22 | 1:28:A:LYS:H | 18 | 0.14 |
| (1,233) | 1:27:A:THR:HG23 | 1:28:A:LYS:H | 18 | 0.14 |
| (1,217) | 1:23:A:GLY:HA3 | 1:42:A:ASN:HD22 | 4 | 0.14 |
| (1,217) | 1:23:A:GLY:HA3 | 1:42:A:ASN:HD22 | 9 | 0.14 |
| (1,185) | 1:11:A:SER:HA | 1:12:A:VAL:H | 1 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 1 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 1 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 1 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 5 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 5 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 5 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 12 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 12 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 12 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 18 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 18 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 18 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 22 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 22 | 0.14 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 22 | 0.14 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 10 | 0.14 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG21 | 17 | 0.14 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG22 | 17 | 0.14 |
| (1,153) | 1:19:A:PRO:HB2 | 1:98:A:THR:HG23 | 17 | 0.14 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 17 | 0.14 |
| (1,108) | 1:70:A:ASP:HB3 | 1:105:A:ARG:HB3 | 5 | 0.14 |
| (1,108) | 1:70:A:ASP:HB3 | 1:105:A:ARG:HB3 | 17 | 0.14 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 15 | 0.14 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 15 | 0.14 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 15 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD11 | 12 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD12 | 12 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD13 | 12 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD11 | 20 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD12 | 20 | 0.14 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD13 | 20 | 0.14 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 3 | 0.14 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 4 | 0.14 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 4 | 0.14 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 4 | 0.14 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 4 | 0.14 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 4 | 0.14 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 4 | 0.14 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 4 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 4 | 0.14 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 4 | 0.14 |
| (1,21) | 1:69:A:CYS:HB3 | 1:71:A:ILE:HG12 | 19 | 0.14 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 2 | 0.13 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 2 | 0.13 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 2 | 0.13 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 20 | 0.13 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 20 | 0.13 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 20 | 0.13 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 3 | 0.13 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 3 | 0.13 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 3 | 0.13 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD11 | 21 | 0.13 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD12 | 21 | 0.13 |
| (1,1602) | 1:40:A:ILE:HA | 1:40:A:ILE:HD13 | 21 | 0.13 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD1 | 10 | 0.13 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD2 | 10 | 0.13 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE1 | 4 | 0.13 |
| (1,1540) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HE2 | 4 | 0.13 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 24 | 0.13 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 24 | 0.13 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 24 | 0.13 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 24 | 0.13 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 24 | 0.13 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 24 | 0.13 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 2 | 0.13 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 2 | 0.13 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 18 | 0.13 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 18 | 0.13 |
| (1,1483) | 1:101:A:PHE:HE1 | 1:102:A:ILE:HG13 | 18 | 0.13 |
| (1,1483) | 1:101:A:PHE:HE2 | 1:102:A:ILE:HG13 | 18 | 0.13 |
| (1,1414) | 1:60:A:HIS:HE1 | 1:92:A:VAL:HB | 17 | 0.13 |
| (1,1414) | 1:60:A:HIS:HE1 | 1:92:A:VAL:HB | 22 | 0.13 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 19 | 0.13 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 19 | 0.13 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 19 | 0.13 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 19 | 0.13 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 19 | 0.13 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 19 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 2 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 2 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 2 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 2 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 2 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 2 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 3 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 3 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 3 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 3 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 3 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 3 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 12 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 12 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 12 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 12 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 12 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 12 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 15 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 15 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 15 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 15 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 15 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 15 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 21 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 21 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 21 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 21 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 21 | 0.13 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 21 | 0.13 |
| (1,1356) | 1:27:A:THR:H | 1:38:A:PHE:HB2 | 14 | 0.13 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 20 | 0.13 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 22 | 0.13 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 22 | 0.13 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 22 | 0.13 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 7 | 0.13 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 7 | 0.13 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 10 | 0.13 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 10 | 0.13 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 13 | 0.13 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 13 | 0.13 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 22 | 0.13 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 22 | 0.13 |
| (1,1269) | 1:27:A:THR:HG21 | 1:29:A:GLY:H | 3 | 0.13 |
| (1,1269) | 1:27:A:THR:HG22 | 1:29:A:GLY:H | 3 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1269) | 1:27:A:THR:HG23 | 1:29:A:GLY:H | 3 | 0.13 |
| (1,1241) | 1:55:A:THR:H | 1:95:A:PRO:HB2 | 1 | 0.13 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 12 | 0.13 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 21 | 0.13 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 7 | 0.13 |
| (1,1191) | 1:46:A:LYS:HB2 | 1:104:A:GLY:H | 19 | 0.13 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 2 | 0.13 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 4 | 0.13 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 8 | 0.13 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 5 | 0.13 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 14 | 0.13 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 20 | 0.13 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 24 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 7 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 7 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 7 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 13 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 13 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 13 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 18 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 18 | 0.13 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 18 | 0.13 |
| (1,1084) | 1:58:A:GLU:H | 1:118:A:LEU:HB3 | 14 | 0.13 |
| (1,1037) | 1:24:A:GLU:H | 1:40:A:ILE:HA | 3 | 0.13 |
| (1,1037) | 1:24:A:GLU:H | 1:40:A:ILE:HA | 22 | 0.13 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 16 | 0.13 |
| (1,957) | 1:32:A:LYS:HD3 | 1:33:A:ASP:H | 9 | 0.13 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 15 | 0.13 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 4 | 0.13 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 4 | 0.13 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 4 | 0.13 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 6 | 0.13 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 6 | 0.13 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 6 | 0.13 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 8 | 0.13 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 8 | 0.13 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 8 | 0.13 |
| (1,882) | 1:64:A:THR:H | 1:112:A:LYS:H | 9 | 0.13 |
| (1,859) | 1:55:A:THR:H | 1:56:A:GLN:HB3 | 4 | 0.13 |
| (1,845) | 1:74:A:LEU:HD11 | 1:103:A:GLU:HB2 | 13 | 0.13 |
| (1,845) | 1:74:A:LEU:HD12 | 1:103:A:GLU:HB2 | 13 | 0.13 |
| (1,845) | 1:74:A:LEU:HD13 | 1:103:A:GLU:HB2 | 13 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,845) | 1:74:A:LEU:HD11 | 1:103:A:GLU:HB2 | 14 | 0.13 |
| (1,845) | 1:74:A:LEU:HD12 | 1:103:A:GLU:HB2 | 14 | 0.13 |
| (1,845) | 1:74:A:LEU:HD13 | 1:103:A:GLU:HB2 | 14 | 0.13 |
| (1,828) | 1:28:A:LYS:HB2 | 1:35:A:GLY:HA3 | 3 | 0.13 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 12 | 0.13 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 12 | 0.13 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 12 | 0.13 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 17 | 0.13 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 17 | 0.13 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 17 | 0.13 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG21 | 5 | 0.13 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG22 | 5 | 0.13 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG23 | 5 | 0.13 |
| (1,812) | 1:62:A:LEU:HB3 | 1:90:A:SER:HA | 4 | 0.13 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 12 | 0.13 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 12 | 0.13 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 12 | 0.13 |
| (1,764) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HB3 | 4 | 0.13 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 7 | 0.13 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 20 | 0.13 |
| (1,713) | 1:126:A:GLN:HA | 1:129:A:LYS:HG3 | 3 | 0.13 |
| (1,682) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HA | 12 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 1 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 15 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 20 | 0.13 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 20 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 20 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 20 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 20 | 0.13 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 20 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 20 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 20 | 0.13 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 20 | 0.13 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 24 | 0.13 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 24 | 0.13 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 24 | 0.13 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 2 | 0.13 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 2 | 0.13 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 2 | 0.13 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 8 | 0.13 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 8 | 0.13 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 8 | 0.13 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 11 | 0.13 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 11 | 0.13 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 11 | 0.13 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 14 | 0.13 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 14 | 0.13 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 14 | 0.13 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 4 | 0.13 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 6 | 0.13 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 16 | 0.13 |
| (1,612) | 1:106:A:VAL:HA | 1:107:A:ASN:HB2 | 4 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 7 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 7 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 7 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 15 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 15 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 15 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 23 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 23 | 0.13 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 23 | 0.13 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 6 | 0.13 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 11 | 0.13 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 12 | 0.13 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 21 | 0.13 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 1 | 0.13 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 8 | 0.13 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 9 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 10 | 0.13 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 11 | 0.13 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 12 | 0.13 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 1 | 0.13 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 2 | 0.13 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 17 | 0.13 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 23 | 0.13 |
| (1,511) | 1:80:A:GLU:HG3 | 1:87:A:TRP:HA | 18 | 0.13 |
| (1,461) | 1:78:A:LYS:HB2 | 1:79:A:LEU:H | 8 | 0.13 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 4 | 0.13 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 16 | 0.13 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 22 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 4 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 4 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 4 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 7 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 7 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 7 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 12 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 12 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 12 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 22 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 22 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 22 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 23 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 23 | 0.13 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 23 | 0.13 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 6 | 0.13 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 6 | 0.13 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 6 | 0.13 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 18 | 0.13 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 18 | 0.13 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 18 | 0.13 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 22 | 0.13 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 22 | 0.13 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 22 | 0.13 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 3 | 0.13 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 13 | 0.13 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 18 | 0.13 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 14 | 0.13 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 14 | 0.13 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 20 | 0.13 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 20 | 0.13 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 20 | 0.13 |
| (1,271) | 1:40:A:ILE:HD11 | 1:51:A:TYR:H | 19 | 0.13 |
| (1,271) | 1:40:A:ILE:HD12 | 1:51:A:TYR:H | 19 | 0.13 |
| (1,271) | 1:40:A:ILE:HD13 | 1:51:A:TYR:H | 19 | 0.13 |
| (1,265) | 1:27:A:THR:HB | 1:39:A:ARG:HB2 | 17 | 0.13 |
| (1,233) | 1:27:A:THR:HG21 | 1:28:A:LYS:H | 21 | 0.13 |
| (1,233) | 1:27:A:THR:HG22 | 1:28:A:LYS:H | 21 | 0.13 |
| (1,233) | 1:27:A:THR:HG23 | 1:28:A:LYS:H | 21 | 0.13 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 2 | 0.13 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 2 | 0.13 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 2 | 0.13 |
| (1,187) | 1:33:A:ASP:HB2 | 1:34:A:ASN:H | 2 | 0.13 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 17 | 0.13 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 17 | 0.13 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 17 | 0.13 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD21 | 10 | 0.13 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD22 | 10 | 0.13 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD23 | 10 | 0.13 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 4 | 0.13 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 16 | 0.13 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 21 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 3 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 3 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 3 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 24 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 24 | 0.13 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 24 | 0.13 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD21 | 2 | 0.13 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD22 | 2 | 0.13 |
| (1,107) | 1:72:A:LYS:HE2 | 1:74:A:LEU:HD23 | 2 | 0.13 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD21 | 2 | 0.13 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD22 | 2 | 0.13 |
| (1,107) | 1:72:A:LYS:HE3 | 1:74:A:LEU:HD23 | 2 | 0.13 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD11 | 17 | 0.13 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD12 | 17 | 0.13 |
| (1,63) | 1:114:A:ASP:HB3 | 1:116:A:LEU:HD13 | 17 | 0.13 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 3 | 0.12 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 3 | 0.12 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 3 | 0.12 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 23 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 23 | 0.12 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 23 | 0.12 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 7 | 0.12 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 7 | 0.12 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 7 | 0.12 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 7 | 0.12 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 7 | 0.12 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 7 | 0.12 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 24 | 0.12 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 24 | 0.12 |
| (1,1513) | 1:94:A:TYR:HB3 | 1:125:A:HIS:HE1 | 3 | 0.12 |
| (1,1513) | 1:94:A:TYR:HB3 | 1:125:A:HIS:HE1 | 22 | 0.12 |
| (1,1512) | 1:125:A:HIS:HD2 | 1:126:A:GLN:HG3 | 23 | 0.12 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE1 | 7 | 0.12 |
| (1,1508) | 1:118:A:LEU:HD21 | 1:122:A:TYR:HE2 | 7 | 0.12 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE1 | 7 | 0.12 |
| (1,1508) | 1:118:A:LEU:HD22 | 1:122:A:TYR:HE2 | 7 | 0.12 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE1 | 7 | 0.12 |
| (1,1508) | 1:118:A:LEU:HD23 | 1:122:A:TYR:HE2 | 7 | 0.12 |
| (1,1483) | 1:101:A:PHE:HE1 | 1:102:A:ILE:HG13 | 1 | 0.12 |
| (1,1483) | 1:101:A:PHE:HE2 | 1:102:A:ILE:HG13 | 1 | 0.12 |
| (1,1483) | 1:101:A:PHE:HE1 | 1:102:A:ILE:HG13 | 3 | 0.12 |
| (1,1483) | 1:101:A:PHE:HE2 | 1:102:A:ILE:HG13 | 3 | 0.12 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 3 | 0.12 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 3 | 0.12 |
| (1,1414) | 1:60:A:HIS:HE1 | 1:92:A:VAL:HB | 12 | 0.12 |
| (1,1387) | 1:14:A:TYR:HD1 | 1:18:A:ARG:HD3 | 5 | 0.12 |
| (1,1387) | 1:14:A:TYR:HD2 | 1:18:A:ARG:HD3 | 5 | 0.12 |
| (1,1387) | 1:14:A:TYR:HD1 | 1:18:A:ARG:HD3 | 12 | 0.12 |
| (1,1387) | 1:14:A:TYR:HD2 | 1:18:A:ARG:HD3 | 12 | 0.12 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 20 | 0.12 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 20 | 0.12 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 20 | 0.12 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 20 | 0.12 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 20 | 0.12 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 20 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 4 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 4 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 4 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 4 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 4 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 4 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 9 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 9 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 9 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 9 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 9 | 0.12 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 9 | 0.12 |
| (1,1375) | 1:56:A:GLN:HG2 | 1:57:A:TYR:HD1 | 11 | 0.12 |
| (1,1375) | 1:56:A:GLN:HG2 | 1:57:A:TYR:HD2 | 11 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 2 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 2 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 4 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 4 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 5 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 5 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 7 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 7 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 15 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 15 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 19 | 0.12 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 19 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG11 | 7 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG12 | 7 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG13 | 7 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG11 | 22 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG12 | 22 | 0.12 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG13 | 22 | 0.12 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 11 | 0.12 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 15 | 0.12 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 23 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 8 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 8 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 8 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 16 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 16 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 16 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG21 | 19 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG22 | 19 | 0.12 |
| (1,1337) | 1:12:A:VAL:H | 1:13:A:THR:HG23 | 19 | 0.12 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 1 | 0.12 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 1 | 0.12 |
| (1,1269) | 1:27:A:THR:HG21 | 1:29:A:GLY:H | 19 | 0.12 |
| (1,1269) | 1:27:A:THR:HG22 | 1:29:A:GLY:H | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1269) | 1:27:A:THR:HG23 | 1:29:A:GLY:H | 19 | 0.12 |
| (1,1269) | 1:27:A:THR:HG21 | 1:29:A:GLY:H | 20 | 0.12 |
| (1,1269) | 1:27:A:THR:HG22 | 1:29:A:GLY:H | 20 | 0.12 |
| (1,1269) | 1:27:A:THR:HG23 | 1:29:A:GLY:H | 20 | 0.12 |
| (1,1266) | 1:74:A:LEU:HD21 | 1:104:A:GLY:H | 7 | 0.12 |
| (1,1266) | 1:74:A:LEU:HD22 | 1:104:A:GLY:H | 7 | 0.12 |
| (1,1266) | 1:74:A:LEU:HD23 | 1:104:A:GLY:H | 7 | 0.12 |
| (1,1263) | 1:70:A:ASP:H | 1:71:A:ILE:HD11 | 16 | 0.12 |
| (1,1263) | 1:70:A:ASP:H | 1:71:A:ILE:HD12 | 16 | 0.12 |
| (1,1263) | 1:70:A:ASP:H | 1:71:A:ILE:HD13 | 16 | 0.12 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 1 | 0.12 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 3 | 0.12 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 9 | 0.12 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 15 | 0.12 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 8 | 0.12 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 14 | 0.12 |
| (1,1211) | 1:28:A:LYS:HB2 | 1:35:A:GLY:H | 3 | 0.12 |
| (1,1211) | 1:28:A:LYS:HB2 | 1:35:A:GLY:H | 9 | 0.12 |
| (1,1211) | 1:28:A:LYS:HB2 | 1:35:A:GLY:H | 15 | 0.12 |
| (1,1191) | 1:46:A:LYS:HB2 | 1:104:A:GLY:H | 20 | 0.12 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 8 | 0.12 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 16 | 0.12 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 20 | 0.12 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 9 | 0.12 |
| (1,1157) | 1:56:A:GLN:HG2 | 1:57:A:TYR:H | 17 | 0.12 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 8 | 0.12 |
| (1,1151) | 1:97:A:GLU:HB3 | 1:98:A:THR:H | 18 | 0.12 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 1 | 0.12 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 6 | 0.12 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 9 | 0.12 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 15 | 0.12 |
| (1,1122) | 1:82:A:GLN:HG2 | 1:86:A:GLU:H | 5 | 0.12 |
| (1,1084) | 1:58:A:GLU:H | 1:118:A:LEU:HB3 | 17 | 0.12 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 22 | 0.12 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 9 | 0.12 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 21 | 0.12 |
| (1,924) | 1:42:A:ASN:H | 1:47:A:GLN:HB2 | 3 | 0.12 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 2 | 0.12 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 2 | 0.12 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 2 | 0.12 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 12 | 0.12 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 12 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 12 | 0.12 |
| (1,859) | 1:55:A:THR:H | 1:56:A:GLN:HB3 | 14 | 0.12 |
| (1,845) | 1:74:A:LEU:HD11 | 1:103:A:GLU:HB2 | 11 | 0.12 |
| (1,845) | 1:74:A:LEU:HD12 | 1:103:A:GLU:HB2 | 11 | 0.12 |
| (1,845) | 1:74:A:LEU:HD13 | 1:103:A:GLU:HB2 | 11 | 0.12 |
| (1,828) | 1:28:A:LYS:HB2 | 1:35:A:GLY:HA3 | 15 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 4 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 4 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 4 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 11 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 11 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 11 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 13 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 13 | 0.12 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 13 | 0.12 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG21 | 24 | 0.12 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG22 | 24 | 0.12 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG23 | 24 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 2 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 2 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 2 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 6 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 6 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 6 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 16 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 16 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 16 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 17 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 17 | 0.12 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 17 | 0.12 |
| (1,758) | 1:126:A:GLN:HA | 1:129:A:LYS:HD3 | 2 | 0.12 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 14 | 0.12 |
| (1,718) | 1:123:A:ARG:HA | 1:126:A:GLN:HG2 | 17 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 6 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 6 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 6 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 9 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 9 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 9 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 17 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 17 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 17 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 19 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 19 | 0.12 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 19 | 0.12 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE1 | 16 | 0.12 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE2 | 16 | 0.12 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE3 | 16 | 0.12 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE1 | 20 | 0.12 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE2 | 20 | 0.12 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE3 | 20 | 0.12 |
| (1,636) | 1:75:A:GLY:H | 1:100:A:MET:HE1 | 21 | 0.12 |
| (1,636) | 1:75:A:GLY:H | 1:100:A:MET:HE2 | 21 | 0.12 |
| (1,636) | 1:75:A:GLY:H | 1:100:A:MET:HE3 | 21 | 0.12 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 7 | 0.12 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 7 | 0.12 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 7 | 0.12 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 16 | 0.12 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 16 | 0.12 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 16 | 0.12 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 3 | 0.12 |
| (1,622) | 1:111:A:SER:HB2 | 1:112:A:LYS:H | 23 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 14 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 15 | 0.12 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 15 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 9 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 9 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 9 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 13 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|----------------|------------------|----------|---------------|
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 13 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 13 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 14 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 14 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 14 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 16 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 16 | 0.12 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 16 | 0.12 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 10 | 0.12 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG21 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG22 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG23 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG21 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG22 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG23 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG21 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG22 | 20 | 0.12 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG23 | 20 | 0.12 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 3 | 0.12 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 6 | 0.12 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 22 | 0.12 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 23 | 0.12 |
| (1,512) | 1:87:A:TRP:HA | 1:88:A:VAL:HB | 12 | 0.12 |
| (1,511) | 1:80:A:GLU:HG3 | 1:87:A:TRP:HA | 20 | 0.12 |
| (1,511) | 1:80:A:GLU:HG3 | 1:87:A:TRP:HA | 23 | 0.12 |
| (1,461) | 1:78:A:LYS:HB2 | 1:79:A:LEU:H | 14 | 0.12 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 14 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 1 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 1 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 1 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 3 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 3 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 3 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 5 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 5 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 5 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 8 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 8 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 8 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 9 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 9 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 9 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 13 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 13 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 13 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 14 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 14 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 14 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 16 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 16 | 0.12 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 16 | 0.12 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 2 | 0.12 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 2 | 0.12 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 2 | 0.12 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 4 | 0.12 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 4 | 0.12 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 4 | 0.12 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 10 | 0.12 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 10 | 0.12 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 10 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB1 | 5 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB2 | 5 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB3 | 5 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB1 | 16 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB2 | 16 | 0.12 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB3 | 16 | 0.12 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 2 | 0.12 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 20 | 0.12 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 21 | 0.12 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG21 | 21 | 0.12 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG22 | 21 | 0.12 |
| (1,293) | 1:40:A:ILE:HG12 | 1:41:A:VAL:HG23 | 21 | 0.12 |
| (1,265) | 1:27:A:THR:HB | 1:39:A:ARG:HB2 | 5 | 0.12 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 14 | 0.12 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 14 | 0.12 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 14 | 0.12 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 16 | 0.12 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 16 | 0.12 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 16 | 0.12 |
| (1,244) | 1:29:A:GLY:HA2 | 1:113:A:MET:HB2 | 4 | 0.12 |
| (1,217) | 1:23:A:GLY:HA3 | 1:42:A:ASN:HD22 | 3 | 0.12 |
| (1,217) | 1:23:A:GLY:HA3 | 1:42:A:ASN:HD22 | 22 | 0.12 |
| (1,205) | 1:15:A:VAL:HG11 | 1:16:A:ASN:H | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,205) | 1:15:A:VAL:HG12 | 1:16:A:ASN:H | 8 | 0.12 |
| (1,205) | 1:15:A:VAL:HG13 | 1:16:A:ASN:H | 8 | 0.12 |
| (1,203) | 1:15:A:VAL:HG21 | 1:16:A:ASN:HB3 | 9 | 0.12 |
| (1,203) | 1:15:A:VAL:HG22 | 1:16:A:ASN:HB3 | 9 | 0.12 |
| (1,203) | 1:15:A:VAL:HG23 | 1:16:A:ASN:HB3 | 9 | 0.12 |
| (1,185) | 1:11:A:SER:HA | 1:12:A:VAL:H | 2 | 0.12 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB1 | 3 | 0.12 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB2 | 3 | 0.12 |
| (1,162) | 1:72:A:LYS:HA | 1:73:A:ALA:HB3 | 3 | 0.12 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 15 | 0.12 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 20 | 0.12 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 9 | 0.12 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 18 | 0.12 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 24 | 0.12 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 24 | 0.12 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 24 | 0.12 |
| (1,90) | 1:19:A:PRO:HA | 1:51:A:TYR:HB2 | 3 | 0.12 |
| (1,78) | 1:55:A:THR:HG21 | 1:95:A:PRO:HB2 | 8 | 0.12 |
| (1,78) | 1:55:A:THR:HG22 | 1:95:A:PRO:HB2 | 8 | 0.12 |
| (1,78) | 1:55:A:THR:HG23 | 1:95:A:PRO:HB2 | 8 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD21 | 13 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD22 | 13 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD23 | 13 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD21 | 14 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD22 | 14 | 0.12 |
| (1,73) | 1:72:A:LYS:HD3 | 1:74:A:LEU:HD23 | 14 | 0.12 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD21 | 20 | 0.12 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD22 | 20 | 0.12 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD23 | 20 | 0.12 |
| (1,43) | 1:76:A:LYS:HG2 | 1:91:A:VAL:HG21 | 13 | 0.12 |
| (1,43) | 1:76:A:LYS:HG2 | 1:91:A:VAL:HG22 | 13 | 0.12 |
| (1,43) | 1:76:A:LYS:HG2 | 1:91:A:VAL:HG23 | 13 | 0.12 |
| (1,25) | 1:89:A:ALA:HB1 | 1:102:A:ILE:HD11 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB1 | 1:102:A:ILE:HD12 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB1 | 1:102:A:ILE:HD13 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB2 | 1:102:A:ILE:HD11 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB2 | 1:102:A:ILE:HD12 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB2 | 1:102:A:ILE:HD13 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB3 | 1:102:A:ILE:HD11 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB3 | 1:102:A:ILE:HD12 | 7 | 0.12 |
| (1,25) | 1:89:A:ALA:HB3 | 1:102:A:ILE:HD13 | 7 | 0.12 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 22 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 22 | 0.12 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 22 | 0.12 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 22 | 0.12 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 22 | 0.12 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 22 | 0.12 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 22 | 0.12 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 22 | 0.12 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 22 | 0.12 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 17 | 0.11 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 17 | 0.11 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 17 | 0.11 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 12 | 0.11 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 12 | 0.11 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 12 | 0.11 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD1 | 23 | 0.11 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD2 | 23 | 0.11 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD11 | 5 | 0.11 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD12 | 5 | 0.11 |
| (1,1519) | 1:94:A:TYR:HD1 | 1:118:A:LEU:HD13 | 5 | 0.11 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD11 | 5 | 0.11 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD12 | 5 | 0.11 |
| (1,1519) | 1:94:A:TYR:HD2 | 1:118:A:LEU:HD13 | 5 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 3 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 3 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 11 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 11 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 12 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 12 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 14 | 0.11 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 14 | 0.11 |
| (1,1504) | 1:51:A:TYR:HE1 | 1:53:A:ASP:HB3 | 13 | 0.11 |
| (1,1504) | 1:51:A:TYR:HE2 | 1:53:A:ASP:HB3 | 13 | 0.11 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 21 | 0.11 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 21 | 0.11 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 21 | 0.11 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 21 | 0.11 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 21 | 0.11 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 21 | 0.11 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 21 | 0.11 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 21 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 5 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 5 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 5 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 5 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 5 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 11 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 11 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 11 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 11 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 11 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 11 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 14 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 14 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 14 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 14 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 14 | 0.11 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 14 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 3 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 3 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 10 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 10 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 14 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 14 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 24 | 0.11 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 24 | 0.11 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG11 | 4 | 0.11 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG12 | 4 | 0.11 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG13 | 4 | 0.11 |
| (1,1356) | 1:27:A:THR:H | 1:38:A:PHE:HB2 | 16 | 0.11 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 8 | 0.11 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 10 | 0.11 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 12 | 0.11 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 21 | 0.11 |
| (1,1297) | 1:54:A:THR:HG21 | 1:56:A:GLN:H | 9 | 0.11 |
| (1,1297) | 1:54:A:THR:HG22 | 1:56:A:GLN:H | 9 | 0.11 |
| (1,1297) | 1:54:A:THR:HG23 | 1:56:A:GLN:H | 9 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 5 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 5 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 11 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 11 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 13 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 13 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 14 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 14 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 19 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 19 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 22 | 0.11 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 22 | 0.11 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 2 | 0.11 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 2 | 0.11 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 16 | 0.11 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 16 | 0.11 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD1 | 17 | 0.11 |
| (1,1287) | 1:93:A:VAL:H | 1:94:A:TYR:HD2 | 17 | 0.11 |
| (1,1278) | 1:100:A:MET:HB3 | 1:102:A:ILE:H | 21 | 0.11 |
| (1,1269) | 1:27:A:THR:HG21 | 1:29:A:GLY:H | 6 | 0.11 |
| (1,1269) | 1:27:A:THR:HG22 | 1:29:A:GLY:H | 6 | 0.11 |
| (1,1269) | 1:27:A:THR:HG23 | 1:29:A:GLY:H | 6 | 0.11 |
| (1,1269) | 1:27:A:THR:HG21 | 1:29:A:GLY:H | 7 | 0.11 |
| (1,1269) | 1:27:A:THR:HG22 | 1:29:A:GLY:H | 7 | 0.11 |
| (1,1269) | 1:27:A:THR:HG23 | 1:29:A:GLY:H | 7 | 0.11 |
| (1,1241) | 1:55:A:THR:H | 1:95:A:PRO:HB2 | 8 | 0.11 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 16 | 0.11 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 17 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 14 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 14 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 14 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD21 | 1:75:A:GLY:H | 15 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD22 | 1:75:A:GLY:H | 15 | 0.11 |
| (1,1230) | 1:74:A:LEU:HD23 | 1:75:A:GLY:H | 15 | 0.11 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 6 | 0.11 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 11 | 0.11 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 13 | 0.11 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 16 | 0.11 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 17 | 0.11 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 21 | 0.11 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 22 | 0.11 |
| (1,1191) | 1:46:A:LYS:HB2 | 1:104:A:GLY:H | 21 | 0.11 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 9 | 0.11 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 14 | 0.11 |
| (1,1177) | 1:68:A:ASP:HA | 1:107:A:ASN:HD21 | 15 | 0.11 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 2 | 0.11 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 19 | 0.11 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 21 | 0.11 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 15 | 0.11 |
| (1,1145) | 1:50:A:TYR:H | 1:101:A:PHE:HB3 | 19 | 0.11 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 5 | 0.11 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 8 | 0.11 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 10 | 0.11 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 13 | 0.11 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 23 | 0.11 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE1 | 3 | 0.11 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE2 | 3 | 0.11 |
| (1,1128) | 1:30:A:PHE:H | 1:113:A:MET:HE3 | 3 | 0.11 |
| (1,1052) | 1:65:A:PHE:HD1 | 1:87:A:TRP:H | 19 | 0.11 |
| (1,1052) | 1:65:A:PHE:HD2 | 1:87:A:TRP:H | 19 | 0.11 |
| (1,1037) | 1:24:A:GLU:H | 1:40:A:ILE:HA | 2 | 0.11 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 2 | 0.11 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 23 | 0.11 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 24 | 0.11 |
| (1,945) | 1:74:A:LEU:H | 1:77:A:THR:H | 21 | 0.11 |
| (1,924) | 1:42:A:ASN:H | 1:47:A:GLN:HB2 | 15 | 0.11 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 7 | 0.11 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 7 | 0.11 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 7 | 0.11 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 11 | 0.11 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 11 | 0.11 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 11 | 0.11 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 17 | 0.11 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 17 | 0.11 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 17 | 0.11 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 22 | 0.11 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 22 | 0.11 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 22 | 0.11 |
| (1,845) | 1:74:A:LEU:HD11 | 1:103:A:GLU:HB2 | 23 | 0.11 |
| (1,845) | 1:74:A:LEU:HD12 | 1:103:A:GLU:HB2 | 23 | 0.11 |
| (1,845) | 1:74:A:LEU:HD13 | 1:103:A:GLU:HB2 | 23 | 0.11 |
| (1,841) | 1:37:A:LEU:HD11 | 1:59:A:MET:H | 21 | 0.11 |
| (1,841) | 1:37:A:LEU:HD12 | 1:59:A:MET:H | 21 | 0.11 |
| (1,841) | 1:37:A:LEU:HD13 | 1:59:A:MET:H | 21 | 0.11 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG21 | 20 | 0.11 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG22 | 20 | 0.11 |
| (1,813) | 1:11:A:SER:HB3 | 1:12:A:VAL:HG23 | 20 | 0.11 |
| (1,812) | 1:62:A:LEU:HB3 | 1:90:A:SER:HA | 16 | 0.11 |
| (1,812) | 1:62:A:LEU:HB3 | 1:90:A:SER:HA | 18 | 0.11 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 21 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 21 | 0.11 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 21 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD21 | 5 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD22 | 5 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD23 | 5 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD21 | 16 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD22 | 16 | 0.11 |
| (1,780) | 1:33:A:ASP:HA | 1:36:A:LEU:HD23 | 16 | 0.11 |
| (1,764) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HB3 | 17 | 0.11 |
| (1,760) | 1:12:A:VAL:HG11 | 1:13:A:THR:HB | 16 | 0.11 |
| (1,760) | 1:12:A:VAL:HG12 | 1:13:A:THR:HB | 16 | 0.11 |
| (1,760) | 1:12:A:VAL:HG13 | 1:13:A:THR:HB | 16 | 0.11 |
| (1,760) | 1:12:A:VAL:HG11 | 1:13:A:THR:HB | 24 | 0.11 |
| (1,760) | 1:12:A:VAL:HG12 | 1:13:A:THR:HB | 24 | 0.11 |
| (1,760) | 1:12:A:VAL:HG13 | 1:13:A:THR:HB | 24 | 0.11 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 13 | 0.11 |
| (1,718) | 1:123:A:ARG:HA | 1:126:A:GLN:HG2 | 1 | 0.11 |
| (1,718) | 1:123:A:ARG:HA | 1:126:A:GLN:HG2 | 4 | 0.11 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE1 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE2 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG21 | 1:113:A:MET:HE3 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE1 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE2 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG22 | 1:113:A:MET:HE3 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE1 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE2 | 3 | 0.11 |
| (1,650) | 1:61:A:VAL:HG23 | 1:113:A:MET:HE3 | 3 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 8 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 8 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 8 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 12 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 12 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 12 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 13 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 13 | 0.11 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 13 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE1 | 8 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE2 | 8 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE3 | 8 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE1 | 21 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE2 | 21 | 0.11 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE3 | 21 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 13 | 0.11 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 13 | 0.11 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 13 | 0.11 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 15 | 0.11 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 15 | 0.11 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 15 | 0.11 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 22 | 0.11 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 22 | 0.11 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 22 | 0.11 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 2 | 0.11 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 6 | 0.11 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 6 | 0.11 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 21 | 0.11 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 21 | 0.11 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 21 | 0.11 |
| (1,563) | 1:97:A:GLU:HG2 | 1:98:A:THR:H | 23 | 0.11 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG21 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG22 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB1 | 1:102:A:ILE:HG23 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG21 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG22 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB2 | 1:102:A:ILE:HG23 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG21 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG22 | 15 | 0.11 |
| (1,549) | 1:73:A:ALA:HB3 | 1:102:A:ILE:HG23 | 15 | 0.11 |
| (1,523) | 1:90:A:SER:HB3 | 1:91:A:VAL:H | 20 | 0.11 |
| (1,523) | 1:90:A:SER:HB3 | 1:91:A:VAL:H | 22 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 4 | 0.11 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 13 | 0.11 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 14 | 0.11 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 15 | 0.11 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 24 | 0.11 |
| (1,511) | 1:80:A:GLU:HG3 | 1:87:A:TRP:HA | 19 | 0.11 |
| (1,493) | 1:83:A:GLU:HG2 | 1:84:A:ASN:H | 9 | 0.11 |
| (1,493) | 1:83:A:GLU:HG3 | 1:84:A:ASN:H | 9 | 0.11 |
| (1,493) | 1:83:A:GLU:HG2 | 1:84:A:ASN:H | 11 | 0.11 |
| (1,493) | 1:83:A:GLU:HG3 | 1:84:A:ASN:H | 11 | 0.11 |
| (1,461) | 1:78:A:LYS:HB2 | 1:79:A:LEU:H | 9 | 0.11 |
| (1,461) | 1:78:A:LYS:HB2 | 1:79:A:LEU:H | 10 | 0.11 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 7 | 0.11 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 9 | 0.11 |
| (1,447) | 1:75:A:GLY:HA2 | 1:100:A:MET:HB3 | 7 | 0.11 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 6 | 0.11 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 6 | 0.11 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 6 | 0.11 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG21 | 24 | 0.11 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG22 | 24 | 0.11 |
| (1,430) | 1:70:A:ASP:H | 1:71:A:ILE:HG23 | 24 | 0.11 |
| (1,321) | 1:49:A:ALA:HB1 | 1:50:A:TYR:HB3 | 17 | 0.11 |
| (1,321) | 1:49:A:ALA:HB2 | 1:50:A:TYR:HB3 | 17 | 0.11 |
| (1,321) | 1:49:A:ALA:HB3 | 1:50:A:TYR:HB3 | 17 | 0.11 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB1 | 7 | 0.11 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB2 | 7 | 0.11 |
| (1,320) | 1:21:A:PHE:HB2 | 1:49:A:ALA:HB3 | 7 | 0.11 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 7 | 0.11 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 10 | 0.11 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 15 | 0.11 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 16 | 0.11 |
| (1,312) | 1:42:A:ASN:H | 1:47:A:GLN:HB3 | 23 | 0.11 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 1 | 0.11 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 1 | 0.11 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 1 | 0.11 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 9 | 0.11 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 9 | 0.11 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 9 | 0.11 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 19 | 0.11 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 19 | 0.11 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 19 | 0.11 |
| (1,233) | 1:27:A:THR:HG21 | 1:28:A:LYS:H | 3 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,233) | 1:27:A:THR:HG22 | 1:28:A:LYS:H | 3 | 0.11 |
| (1,233) | 1:27:A:THR:HG23 | 1:28:A:LYS:H | 3 | 0.11 |
| (1,217) | 1:23:A:GLY:HA3 | 1:42:A:ASN:HD22 | 7 | 0.11 |
| (1,205) | 1:15:A:VAL:HG11 | 1:16:A:ASN:H | 1 | 0.11 |
| (1,205) | 1:15:A:VAL:HG12 | 1:16:A:ASN:H | 1 | 0.11 |
| (1,205) | 1:15:A:VAL:HG13 | 1:16:A:ASN:H | 1 | 0.11 |
| (1,205) | 1:15:A:VAL:HG11 | 1:16:A:ASN:H | 3 | 0.11 |
| (1,205) | 1:15:A:VAL:HG12 | 1:16:A:ASN:H | 3 | 0.11 |
| (1,205) | 1:15:A:VAL:HG13 | 1:16:A:ASN:H | 3 | 0.11 |
| (1,205) | 1:15:A:VAL:HG11 | 1:16:A:ASN:H | 24 | 0.11 |
| (1,205) | 1:15:A:VAL:HG12 | 1:16:A:ASN:H | 24 | 0.11 |
| (1,205) | 1:15:A:VAL:HG13 | 1:16:A:ASN:H | 24 | 0.11 |
| (1,199) | 1:50:A:TYR:H | 1:98:A:THR:HG21 | 11 | 0.11 |
| (1,199) | 1:50:A:TYR:H | 1:98:A:THR:HG22 | 11 | 0.11 |
| (1,199) | 1:50:A:TYR:H | 1:98:A:THR:HG23 | 11 | 0.11 |
| (1,187) | 1:33:A:ASP:HB2 | 1:34:A:ASN:H | 16 | 0.11 |
| (1,185) | 1:11:A:SER:HA | 1:12:A:VAL:H | 16 | 0.11 |
| (1,160) | 1:18:A:ARG:HB2 | 1:19:A:PRO:HD3 | 1 | 0.11 |
| (1,129) | 1:71:A:ILE:HG21 | 1:102:A:ILE:HD11 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG21 | 1:102:A:ILE:HD12 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG21 | 1:102:A:ILE:HD13 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG22 | 1:102:A:ILE:HD11 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG22 | 1:102:A:ILE:HD12 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG22 | 1:102:A:ILE:HD13 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG23 | 1:102:A:ILE:HD11 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG23 | 1:102:A:ILE:HD12 | 22 | 0.11 |
| (1,129) | 1:71:A:ILE:HG23 | 1:102:A:ILE:HD13 | 22 | 0.11 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 10 | 0.11 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 13 | 0.11 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 22 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 9 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 9 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 9 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 17 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 17 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 17 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 18 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 18 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 18 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG21 | 21 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG22 | 21 | 0.11 |
| (1,115) | 1:23:A:GLY:HA2 | 1:40:A:ILE:HG23 | 21 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 19 | 0.11 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 19 | 0.11 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 19 | 0.11 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 23 | 0.11 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 23 | 0.11 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 23 | 0.11 |
| (1,90) | 1:19:A:PRO:HA | 1:51:A:TYR:HB2 | 5 | 0.11 |
| (1,90) | 1:19:A:PRO:HA | 1:51:A:TYR:HB2 | 23 | 0.11 |
| (1,78) | 1:55:A:THR:HG21 | 1:95:A:PRO:HB2 | 3 | 0.11 |
| (1,78) | 1:55:A:THR:HG22 | 1:95:A:PRO:HB2 | 3 | 0.11 |
| (1,78) | 1:55:A:THR:HG23 | 1:95:A:PRO:HB2 | 3 | 0.11 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD21 | 12 | 0.11 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD22 | 12 | 0.11 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD23 | 12 | 0.11 |
| (1,40) | 1:91:A:VAL:HG21 | 1:99:A:GLU:HB3 | 5 | 0.11 |
| (1,40) | 1:91:A:VAL:HG22 | 1:99:A:GLU:HB3 | 5 | 0.11 |
| (1,40) | 1:91:A:VAL:HG23 | 1:99:A:GLU:HB3 | 5 | 0.11 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 8 | 0.11 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 16 | 0.11 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 16 | 0.11 |
| (1,19) | 1:116:A:LEU:HD11 | 1:117:A:PRO:HD3 | 19 | 0.11 |
| (1,19) | 1:116:A:LEU:HD12 | 1:117:A:PRO:HD3 | 19 | 0.11 |
| (1,19) | 1:116:A:LEU:HD13 | 1:117:A:PRO:HD3 | 19 | 0.11 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 11 | 0.1 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 11 | 0.1 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 11 | 0.1 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD21 | 14 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD22 | 14 | 0.1 |
| (1,1668) | 1:60:A:HIS:HE1 | 1:116:A:LEU:HD23 | 14 | 0.1 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG11 | 7 | 0.1 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG12 | 7 | 0.1 |
| (1,1651) | 1:106:A:VAL:H | 1:106:A:VAL:HG13 | 7 | 0.1 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD1 | 18 | 0.1 |
| (1,1586) | 1:12:A:VAL:HB | 1:14:A:TYR:HD2 | 18 | 0.1 |
| (1,1574) | 1:68:A:ASP:H | 1:69:A:CYS:H | 19 | 0.1 |
| (1,1533) | 1:46:A:LYS:HE3 | 1:48:A:TRP:HD1 | 2 | 0.1 |
| (1,1533) | 1:46:A:LYS:HE3 | 1:48:A:TRP:HD1 | 13 | 0.1 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD1 | 6 | 0.1 |
| (1,1518) | 1:94:A:TYR:HA | 1:122:A:TYR:HD2 | 6 | 0.1 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD1 | 22 | 0.1 |
| (1,1517) | 1:94:A:TYR:HB2 | 1:122:A:TYR:HD2 | 22 | 0.1 |
| (1,1514) | 1:125:A:HIS:HE1 | 1:129:A:LYS:HD3 | 18 | 0.1 |
| (1,1504) | 1:51:A:TYR:HE1 | 1:53:A:ASP:HB3 | 1 | 0.1 |
| (1,1504) | 1:51:A:TYR:HE2 | 1:53:A:ASP:HB3 | 1 | 0.1 |
| (1,1436) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HD2 | 5 | 0.1 |
| (1,1436) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HD2 | 5 | 0.1 |
| (1,1435) | 1:14:A:TYR:HE1 | 1:19:A:PRO:HG2 | 10 | 0.1 |
| (1,1435) | 1:14:A:TYR:HE2 | 1:19:A:PRO:HG2 | 10 | 0.1 |
| (1,1433) | 1:14:A:TYR:HE1 | 1:38:A:PHE:HB2 | 8 | 0.1 |
| (1,1433) | 1:14:A:TYR:HE2 | 1:38:A:PHE:HB2 | 8 | 0.1 |
| (1,1414) | 1:60:A:HIS:HE1 | 1:92:A:VAL:HB | 4 | 0.1 |
| (1,1414) | 1:60:A:HIS:HE1 | 1:92:A:VAL:HB | 6 | 0.1 |
| (1,1414) | 1:60:A:HIS:HE1 | 1:92:A:VAL:HB | 8 | 0.1 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG21 | 5 | 0.1 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG22 | 5 | 0.1 |
| (1,1383) | 1:50:A:TYR:HD1 | 1:93:A:VAL:HG23 | 5 | 0.1 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG21 | 5 | 0.1 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG22 | 5 | 0.1 |
| (1,1383) | 1:50:A:TYR:HD2 | 1:93:A:VAL:HG23 | 5 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 16 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 16 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 16 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 16 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 16 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 16 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 22 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 22 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 22 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 22 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 22 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 22 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB1 | 24 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB2 | 24 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD1 | 1:115:A:ALA:HB3 | 24 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB1 | 24 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB2 | 24 | 0.1 |
| (1,1377) | 1:57:A:TYR:HD2 | 1:115:A:ALA:HB3 | 24 | 0.1 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 11 | 0.1 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 11 | 0.1 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD1 | 22 | 0.1 |
| (1,1373) | 1:54:A:THR:HA | 1:57:A:TYR:HD2 | 22 | 0.1 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG11 | 8 | 0.1 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG12 | 8 | 0.1 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG13 | 8 | 0.1 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG11 | 12 | 0.1 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG12 | 12 | 0.1 |
| (1,1363) | 1:48:A:TRP:HZ2 | 1:106:A:VAL:HG13 | 12 | 0.1 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 5 | 0.1 |
| (1,1343) | 1:15:A:VAL:HB | 1:17:A:GLY:H | 13 | 0.1 |
| (1,1313) | 1:106:A:VAL:HB | 1:108:A:GLY:H | 7 | 0.1 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD1 | 12 | 0.1 |
| (1,1294) | 1:118:A:LEU:H | 1:122:A:TYR:HD2 | 12 | 0.1 |
| (1,1266) | 1:74:A:LEU:HD21 | 1:104:A:GLY:H | 16 | 0.1 |
| (1,1266) | 1:74:A:LEU:HD22 | 1:104:A:GLY:H | 16 | 0.1 |
| (1,1266) | 1:74:A:LEU:HD23 | 1:104:A:GLY:H | 16 | 0.1 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 6 | 0.1 |
| (1,1237) | 1:12:A:VAL:H | 1:13:A:THR:H | 20 | 0.1 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 9 | 0.1 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 12 | 0.1 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 15 | 0.1 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 20 | 0.1 |
| (1,1227) | 1:101:A:PHE:HB3 | 1:102:A:ILE:H | 24 | 0.1 |
| (1,1191) | 1:46:A:LYS:HB2 | 1:104:A:GLY:H | 17 | 0.1 |
| (1,1165) | 1:77:A:THR:HA | 1:90:A:SER:H | 16 | 0.1 |
| (1,1163) | 1:79:A:LEU:HA | 1:90:A:SER:H | 14 | 0.1 |
| (1,1133) | 1:69:A:CYS:H | 1:71:A:ILE:H | 2 | 0.1 |
| (1,1037) | 1:24:A:GLU:H | 1:40:A:ILE:HA | 24 | 0.1 |
| (1,1018) | 1:52:A:ASN:HB3 | 1:97:A:GLU:H | 6 | 0.1 |
| (1,952) | 1:72:A:LYS:HB3 | 1:73:A:ALA:H | 8 | 0.1 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 1 | 0.1 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 1 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 1 | 0.1 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 13 | 0.1 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 13 | 0.1 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 13 | 0.1 |
| (1,902) | 1:26:A:VAL:HG11 | 1:41:A:VAL:H | 14 | 0.1 |
| (1,902) | 1:26:A:VAL:HG12 | 1:41:A:VAL:H | 14 | 0.1 |
| (1,902) | 1:26:A:VAL:HG13 | 1:41:A:VAL:H | 14 | 0.1 |
| (1,859) | 1:55:A:THR:H | 1:56:A:GLN:HB3 | 7 | 0.1 |
| (1,845) | 1:74:A:LEU:HD11 | 1:103:A:GLU:HB2 | 9 | 0.1 |
| (1,845) | 1:74:A:LEU:HD12 | 1:103:A:GLU:HB2 | 9 | 0.1 |
| (1,845) | 1:74:A:LEU:HD13 | 1:103:A:GLU:HB2 | 9 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 1 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 1 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 1 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 2 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 2 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 2 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG21 | 9 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG22 | 9 | 0.1 |
| (1,814) | 1:25:A:GLU:HG3 | 1:27:A:THR:HG23 | 9 | 0.1 |
| (1,812) | 1:62:A:LEU:HB3 | 1:90:A:SER:HA | 8 | 0.1 |
| (1,804) | 1:62:A:LEU:HD21 | 1:112:A:LYS:H | 5 | 0.1 |
| (1,804) | 1:62:A:LEU:HD22 | 1:112:A:LYS:H | 5 | 0.1 |
| (1,804) | 1:62:A:LEU:HD23 | 1:112:A:LYS:H | 5 | 0.1 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD11 | 20 | 0.1 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD12 | 20 | 0.1 |
| (1,792) | 1:47:A:GLN:HG2 | 1:74:A:LEU:HD13 | 20 | 0.1 |
| (1,764) | 1:19:A:PRO:HB2 | 1:51:A:TYR:HB3 | 7 | 0.1 |
| (1,723) | 1:129:A:LYS:HA | 1:130:A:ASP:H | 23 | 0.1 |
| (1,718) | 1:123:A:ARG:HA | 1:126:A:GLN:HG2 | 13 | 0.1 |
| (1,718) | 1:123:A:ARG:HA | 1:126:A:GLN:HG2 | 21 | 0.1 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE1 | 4 | 0.1 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE2 | 4 | 0.1 |
| (1,649) | 1:111:A:SER:HB3 | 1:113:A:MET:HE3 | 4 | 0.1 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE1 | 14 | 0.1 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE2 | 14 | 0.1 |
| (1,639) | 1:37:A:LEU:HA | 1:59:A:MET:HE3 | 14 | 0.1 |
| (1,624) | 1:63:A:VAL:HG21 | 1:111:A:SER:HB2 | 4 | 0.1 |
| (1,624) | 1:63:A:VAL:HG22 | 1:111:A:SER:HB2 | 4 | 0.1 |
| (1,624) | 1:63:A:VAL:HG23 | 1:111:A:SER:HB2 | 4 | 0.1 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG11 | 20 | 0.1 |
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG12 | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,595) | 1:102:A:ILE:HD11 | 1:106:A:VAL:HG13 | 20 | 0.1 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG11 | 20 | 0.1 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG12 | 20 | 0.1 |
| (1,595) | 1:102:A:ILE:HD12 | 1:106:A:VAL:HG13 | 20 | 0.1 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG11 | 20 | 0.1 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG12 | 20 | 0.1 |
| (1,595) | 1:102:A:ILE:HD13 | 1:106:A:VAL:HG13 | 20 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 5 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 5 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 5 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 20 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 20 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 20 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD11 | 22 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD12 | 22 | 0.1 |
| (1,586) | 1:48:A:TRP:HA | 1:102:A:ILE:HD13 | 22 | 0.1 |
| (1,515) | 1:65:A:PHE:HB3 | 1:87:A:TRP:HB3 | 2 | 0.1 |
| (1,493) | 1:83:A:GLU:HG2 | 1:84:A:ASN:H | 2 | 0.1 |
| (1,493) | 1:83:A:GLU:HG3 | 1:84:A:ASN:H | 2 | 0.1 |
| (1,493) | 1:83:A:GLU:HG2 | 1:84:A:ASN:H | 6 | 0.1 |
| (1,493) | 1:83:A:GLU:HG3 | 1:84:A:ASN:H | 6 | 0.1 |
| (1,493) | 1:83:A:GLU:HG2 | 1:84:A:ASN:H | 17 | 0.1 |
| (1,493) | 1:83:A:GLU:HG3 | 1:84:A:ASN:H | 17 | 0.1 |
| (1,493) | 1:83:A:GLU:HG2 | 1:84:A:ASN:H | 20 | 0.1 |
| (1,493) | 1:83:A:GLU:HG3 | 1:84:A:ASN:H | 20 | 0.1 |
| (1,461) | 1:78:A:LYS:HB2 | 1:79:A:LEU:H | 23 | 0.1 |
| (1,454) | 1:76:A:LYS:HD3 | 1:77:A:THR:HA | 15 | 0.1 |
| (1,354) | 1:37:A:LEU:HD21 | 1:59:A:MET:HA | 9 | 0.1 |
| (1,354) | 1:37:A:LEU:HD22 | 1:59:A:MET:HA | 9 | 0.1 |
| (1,354) | 1:37:A:LEU:HD23 | 1:59:A:MET:HA | 9 | 0.1 |
| (1,271) | 1:40:A:ILE:HD11 | 1:51:A:TYR:H | 16 | 0.1 |
| (1,271) | 1:40:A:ILE:HD12 | 1:51:A:TYR:H | 16 | 0.1 |
| (1,271) | 1:40:A:ILE:HD13 | 1:51:A:TYR:H | 16 | 0.1 |
| (1,265) | 1:27:A:THR:HB | 1:39:A:ARG:HB2 | 4 | 0.1 |
| (1,253) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB2 | 24 | 0.1 |
| (1,253) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB2 | 24 | 0.1 |
| (1,253) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB2 | 24 | 0.1 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 4 | 0.1 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 4 | 0.1 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 4 | 0.1 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 17 | 0.1 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 17 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 17 | 0.1 |
| (1,252) | 1:15:A:VAL:HG21 | 1:34:A:ASN:HB3 | 20 | 0.1 |
| (1,252) | 1:15:A:VAL:HG22 | 1:34:A:ASN:HB3 | 20 | 0.1 |
| (1,252) | 1:15:A:VAL:HG23 | 1:34:A:ASN:HB3 | 20 | 0.1 |
| (1,233) | 1:27:A:THR:HG21 | 1:28:A:LYS:H | 19 | 0.1 |
| (1,233) | 1:27:A:THR:HG22 | 1:28:A:LYS:H | 19 | 0.1 |
| (1,233) | 1:27:A:THR:HG23 | 1:28:A:LYS:H | 19 | 0.1 |
| (1,214) | 1:22:A:VAL:HG11 | 1:23:A:GLY:H | 17 | 0.1 |
| (1,214) | 1:22:A:VAL:HG12 | 1:23:A:GLY:H | 17 | 0.1 |
| (1,214) | 1:22:A:VAL:HG13 | 1:23:A:GLY:H | 17 | 0.1 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD21 | 8 | 0.1 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD22 | 8 | 0.1 |
| (1,145) | 1:56:A:GLN:HA | 1:118:A:LEU:HD23 | 8 | 0.1 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 2 | 0.1 |
| (1,127) | 1:69:A:CYS:HB2 | 1:106:A:VAL:HA | 23 | 0.1 |
| (1,99) | 1:73:A:ALA:HB1 | 1:79:A:LEU:HG | 6 | 0.1 |
| (1,99) | 1:73:A:ALA:HB2 | 1:79:A:LEU:HG | 6 | 0.1 |
| (1,99) | 1:73:A:ALA:HB3 | 1:79:A:LEU:HG | 6 | 0.1 |
| (1,90) | 1:19:A:PRO:HA | 1:51:A:TYR:HB2 | 10 | 0.1 |
| (1,78) | 1:55:A:THR:HG21 | 1:95:A:PRO:HB2 | 24 | 0.1 |
| (1,78) | 1:55:A:THR:HG22 | 1:95:A:PRO:HB2 | 24 | 0.1 |
| (1,78) | 1:55:A:THR:HG23 | 1:95:A:PRO:HB2 | 24 | 0.1 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD21 | 22 | 0.1 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD22 | 22 | 0.1 |
| (1,58) | 1:58:A:GLU:HG3 | 1:118:A:LEU:HD23 | 22 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 6 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 10 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|--------|------------------|-----------------|----------|---------------|
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 10 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 14 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB1 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB2 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG11 | 1:89:A:ALA:HB3 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB1 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB2 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG12 | 1:89:A:ALA:HB3 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB1 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB2 | 20 | 0.1 |
| (1,23) | 1:63:A:VAL:HG13 | 1:89:A:ALA:HB3 | 20 | 0.1 |
| (1,19) | 1:116:A:LEU:HD11 | 1:117:A:PRO:HD3 | 1 | 0.1 |
| (1,19) | 1:116:A:LEU:HD12 | 1:117:A:PRO:HD3 | 1 | 0.1 |
| (1,19) | 1:116:A:LEU:HD13 | 1:117:A:PRO:HD3 | 1 | 0.1 |
| (1,19) | 1:116:A:LEU:HD11 | 1:117:A:PRO:HD3 | 10 | 0.1 |
| (1,19) | 1:116:A:LEU:HD12 | 1:117:A:PRO:HD3 | 10 | 0.1 |
| (1,19) | 1:116:A:LEU:HD13 | 1:117:A:PRO:HD3 | 10 | 0.1 |
| (1,19) | 1:116:A:LEU:HD11 | 1:117:A:PRO:HD3 | 23 | 0.1 |
| (1,19) | 1:116:A:LEU:HD12 | 1:117:A:PRO:HD3 | 23 | 0.1 |
| (1,19) | 1:116:A:LEU:HD13 | 1:117:A:PRO:HD3 | 23 | 0.1 |

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

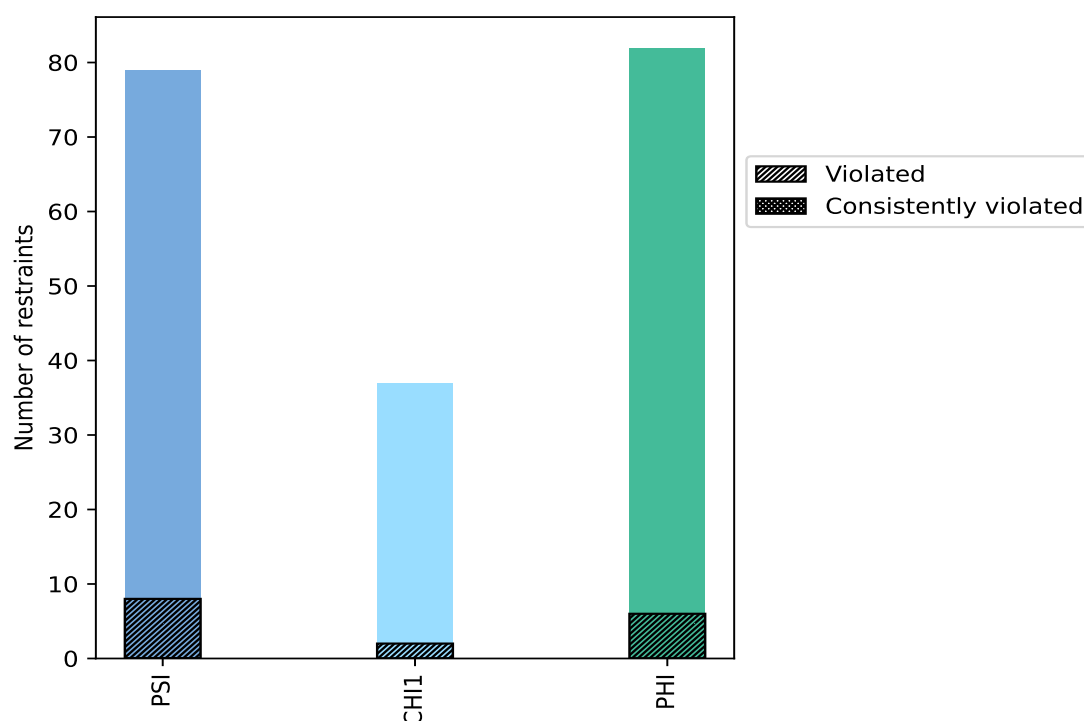
10.1 Summary of dihedral-angle violations [i](#)

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 | 79 | 39.9 | 8 | 10.1 | 4.0 | 0 | 0.0 | 0.0 |
| CHI1 | 37 | 18.7 | 2 | 5.4 | 1.0 | 0 | 0.0 | 0.0 |
| PHI | 82 | 41.4 | 6 | 7.3 | 3.0 | 0 | 0.0 | 0.0 |
| Total | 198 | 100.0 | 16 | 8.1 | 8.1 | 0 | 0.0 | 0.0 |

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

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



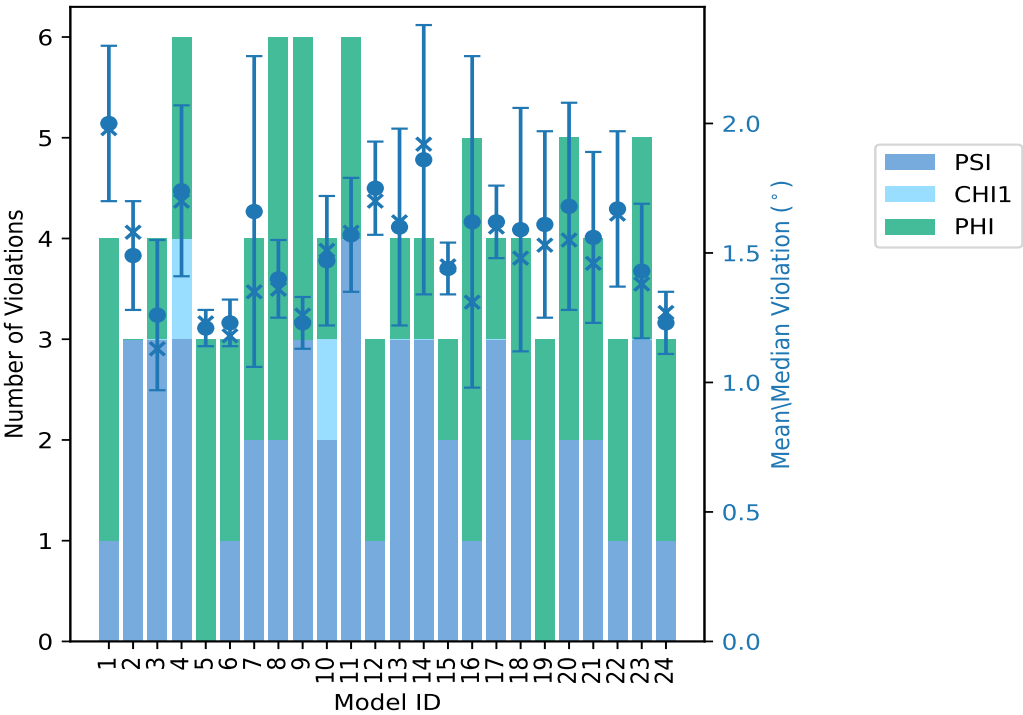
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

| Model ID | Number of violations | | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|------|-----|-------|----------|---------|--------|------------|
| | PSI | CHI1 | PHI | Total | | | | |
| 1 | 1 | 0 | 3 | 4 | 2.0 | 2.43 | 0.3 | 1.98 |
| 2 | 3 | 0 | 0 | 3 | 1.49 | 1.69 | 0.21 | 1.58 |
| 3 | 3 | 0 | 1 | 4 | 1.26 | 1.76 | 0.29 | 1.13 |
| 4 | 3 | 1 | 2 | 6 | 1.74 | 2.15 | 0.33 | 1.7 |
| 5 | 0 | 0 | 3 | 3 | 1.21 | 1.29 | 0.07 | 1.23 |
| 6 | 1 | 0 | 2 | 3 | 1.23 | 1.35 | 0.09 | 1.18 |
| 7 | 2 | 0 | 2 | 4 | 1.66 | 2.69 | 0.6 | 1.35 |
| 8 | 2 | 0 | 4 | 6 | 1.4 | 1.68 | 0.15 | 1.36 |
| 9 | 3 | 0 | 3 | 6 | 1.23 | 1.33 | 0.1 | 1.26 |
| 10 | 2 | 1 | 1 | 4 | 1.47 | 1.78 | 0.25 | 1.51 |
| 11 | 4 | 0 | 2 | 6 | 1.57 | 1.98 | 0.22 | 1.58 |
| 12 | 1 | 0 | 2 | 3 | 1.75 | 1.99 | 0.18 | 1.7 |
| 13 | 3 | 0 | 1 | 4 | 1.6 | 2.0 | 0.38 | 1.62 |
| 14 | 3 | 0 | 1 | 4 | 1.86 | 2.38 | 0.52 | 1.92 |
| 15 | 2 | 0 | 1 | 3 | 1.44 | 1.56 | 0.1 | 1.45 |
| 16 | 1 | 0 | 4 | 5 | 1.62 | 2.6 | 0.64 | 1.31 |
| 17 | 3 | 0 | 1 | 4 | 1.62 | 1.84 | 0.14 | 1.6 |
| 18 | 2 | 0 | 2 | 4 | 1.59 | 2.32 | 0.47 | 1.48 |
| 19 | 0 | 0 | 3 | 3 | 1.61 | 2.09 | 0.36 | 1.53 |
| 20 | 2 | 0 | 3 | 5 | 1.68 | 2.45 | 0.4 | 1.55 |
| 21 | 2 | 0 | 2 | 4 | 1.56 | 2.09 | 0.33 | 1.46 |
| 22 | 1 | 0 | 2 | 3 | 1.67 | 2.05 | 0.3 | 1.65 |
| 23 | 3 | 0 | 2 | 5 | 1.43 | 1.78 | 0.26 | 1.38 |
| 24 | 1 | 0 | 2 | 3 | 1.23 | 1.36 | 0.12 | 1.27 |

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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

| Number of violated restraints | | | | Fraction of the ensemble | |
|-------------------------------|------|-----|-------|--------------------------|------|
| PSI | CHI1 | PHI | Total | Count ¹ | % |
| 2 | 2 | 1 | 5 | 1 | 4.2 |
| 1 | 0 | 0 | 1 | 2 | 8.3 |
| 0 | 0 | 0 | 0 | 3 | 12.5 |
| 0 | 0 | 0 | 0 | 4 | 16.7 |
| 1 | 0 | 0 | 1 | 5 | 20.8 |
| 1 | 0 | 0 | 1 | 6 | 25.0 |
| 0 | 0 | 1 | 1 | 7 | 29.2 |
| 1 | 0 | 2 | 3 | 8 | 33.3 |
| 0 | 0 | 1 | 1 | 9 | 37.5 |
| 0 | 0 | 0 | 0 | 10 | 41.7 |
| 1 | 0 | 0 | 1 | 11 | 45.8 |

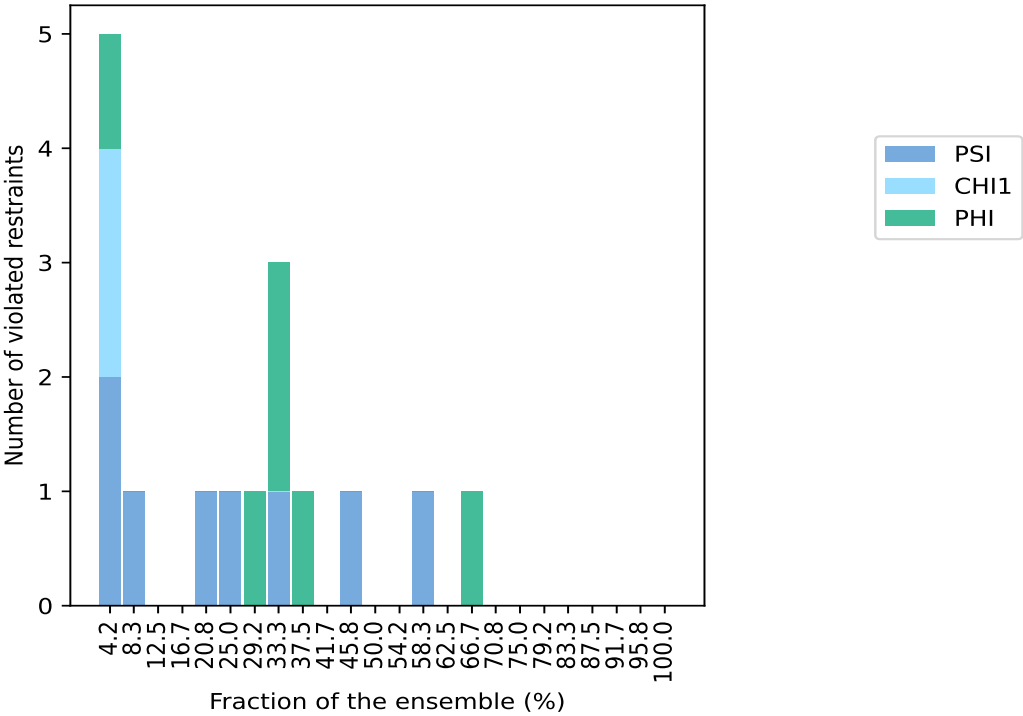
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| Number of violated restraints | | | | Fraction of the ensemble | |
|-------------------------------|------|-----|-------|--------------------------|-------|
| PSI | CHI1 | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 0 | 12 | 50.0 |
| 0 | 0 | 0 | 0 | 13 | 54.2 |
| 1 | 0 | 0 | 1 | 14 | 58.3 |
| 0 | 0 | 0 | 0 | 15 | 62.5 |
| 0 | 0 | 1 | 1 | 16 | 66.7 |
| 0 | 0 | 0 | 0 | 17 | 70.8 |
| 0 | 0 | 0 | 0 | 18 | 75.0 |
| 0 | 0 | 0 | 0 | 19 | 79.2 |
| 0 | 0 | 0 | 0 | 20 | 83.3 |
| 0 | 0 | 0 | 0 | 21 | 87.5 |
| 0 | 0 | 0 | 0 | 22 | 91.7 |
| 0 | 0 | 0 | 0 | 23 | 95.8 |
| 0 | 0 | 0 | 0 | 24 | 100.0 |

¹ Number of models with violations

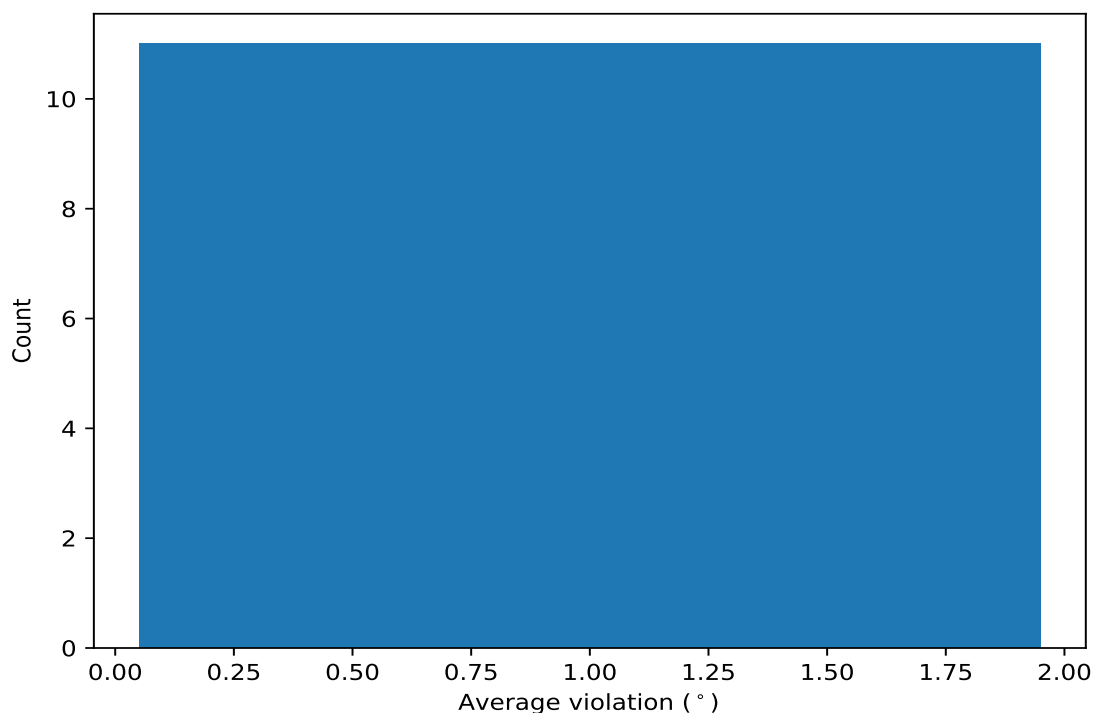
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble ⓘ



10.4 Most violated dihedral-angle restraints in the ensemble [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.

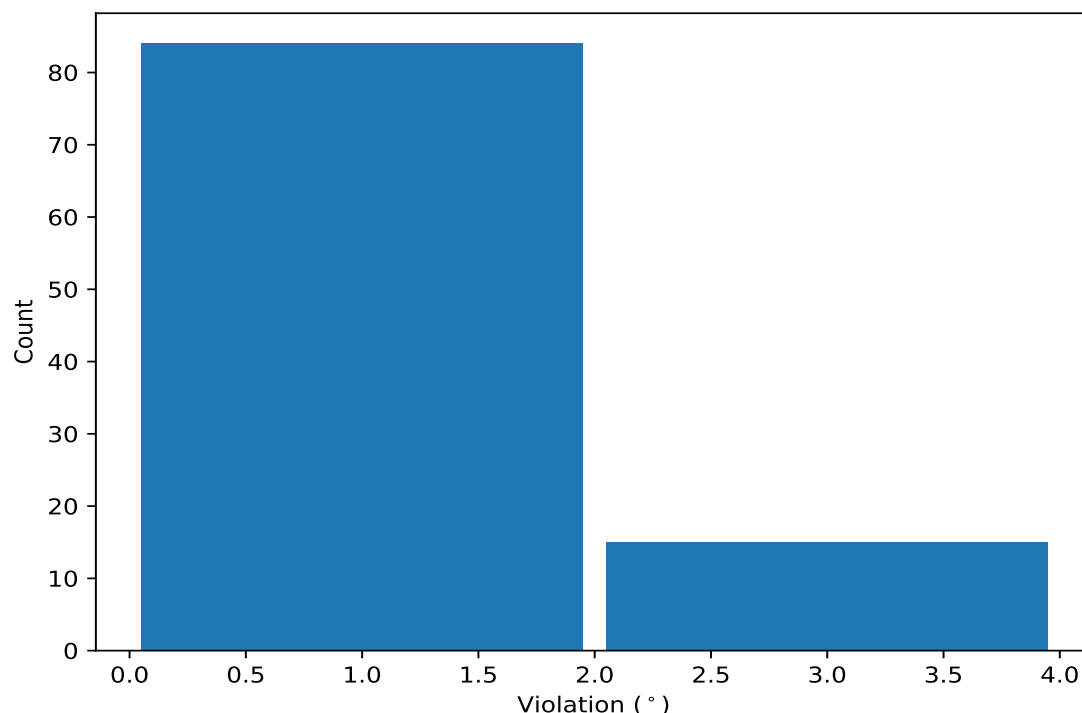
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 16 | 1.88 | 0.43 | 1.97 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 14 | 1.33 | 0.2 | 1.23 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 11 | 1.51 | 0.22 | 1.46 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 9 | 1.4 | 0.25 | 1.35 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 8 | 1.91 | 0.55 | 1.82 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 8 | 1.51 | 0.36 | 1.33 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 8 | 1.42 | 0.33 | 1.4 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 7 | 1.58 | 0.27 | 1.6 |
| (1,116) | 1:100:A:MET:N | 1:100:A:MET:CA | 1:100:A:MET:C | 1:101:A:PHE:N | 6 | 1.35 | 0.2 | 1.34 |
| (1,139) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:LEU:N | 5 | 1.49 | 0.22 | 1.56 |
| (1,18) | 1:27:A:THR:N | 1:27:A:THR:CA | 1:27:A:THR:C | 1:28:A:LYS:N | 2 | 1.42 | 0.16 | 1.42 |

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 (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 7 | 2.69 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 16 | 2.6 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 20 | 2.45 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 1 | 2.43 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 14 | 2.38 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 14 | 2.37 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 18 | 2.32 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 4 | 2.15 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 4 | 2.13 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 16 | 2.13 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 19 | 2.09 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 21 | 2.09 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 22 | 2.05 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 1 | 2.04 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 13 | 2.0 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 12 | 1.99 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 11 | 1.98 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 13 | 1.95 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 1 | 1.93 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 17 | 1.84 |
| (1,167) | 1:42:A:ASN:N | 1:42:A:ASN:CA | 1:42:A:ASN:CB | 1:42:A:ASN:CG | 4 | 1.8 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 10 | 1.78 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 23 | 1.78 |
| (1,139) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:LEU:N | 3 | 1.76 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 12 | 1.7 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 2 | 1.69 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 18 | 1.69 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 8 | 1.68 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 23 | 1.67 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 22 | 1.65 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 20 | 1.65 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 17 | 1.64 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 11 | 1.6 |
| (1,116) | 1:100:A:MET:N | 1:100:A:MET:CA | 1:100:A:MET:C | 1:101:A:PHE:N | 4 | 1.59 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 11 | 1.59 |
| (1,139) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:LEU:N | 2 | 1.58 |
| (1,116) | 1:100:A:MET:N | 1:100:A:MET:CA | 1:100:A:MET:C | 1:101:A:PHE:N | 1 | 1.58 |
| (1,18) | 1:27:A:THR:N | 1:27:A:THR:CA | 1:27:A:THR:C | 1:28:A:LYS:N | 21 | 1.58 |
| (1,139) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:LEU:N | 15 | 1.56 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 4 | 1.56 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 11 | 1.56 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 12 | 1.55 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 10 | 1.55 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 17 | 1.55 |
| (1,20) | 1:28:A:LYS:N | 1:28:A:LYS:CA | 1:28:A:LYS:C | 1:29:A:GLY:N | 20 | 1.55 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 19 | 1.53 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 8 | 1.51 |
| (1,139) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:LEU:N | 10 | 1.47 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 14 | 1.46 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 11 | 1.46 |
| (1,116) | 1:100:A:MET:N | 1:100:A:MET:CA | 1:100:A:MET:C | 1:101:A:PHE:N | 17 | 1.45 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 20 | 1.45 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 15 | 1.45 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 7 | 1.42 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 23 | 1.38 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 8 | 1.38 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 24 | 1.36 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 21 | 1.35 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 6 | 1.35 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 8 | 1.34 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 9 | 1.33 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 8 | 1.32 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 20 | 1.32 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 15 | 1.31 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 22 | 1.31 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|---------------|---------------|----------|---------------|
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 9 | 1.31 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 16 | 1.31 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 5 | 1.29 |
| (1,121) | 1:103:A:GLU:N | 1:103:A:GLU:CA | 1:103:A:GLU:C | 1:104:A:GLY:N | 13 | 1.28 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 7 | 1.28 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 24 | 1.27 |
| (1,18) | 1:27:A:THR:N | 1:27:A:THR:CA | 1:27:A:THR:C | 1:28:A:LYS:N | 18 | 1.27 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 9 | 1.26 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 9 | 1.26 |
| (1,116) | 1:100:A:MET:N | 1:100:A:MET:CA | 1:100:A:MET:C | 1:101:A:PHE:N | 21 | 1.24 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 7 | 1.24 |
| (1,80) | 1:72:A:LYS:N | 1:72:A:LYS:CA | 1:72:A:LYS:C | 1:73:A:ALA:N | 11 | 1.24 |
| (1,68) | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 1:63:A:VAL:N | 14 | 1.24 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 4 | 1.23 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 5 | 1.23 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 19 | 1.21 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 2 | 1.2 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 23 | 1.2 |
| (1,54) | 1:53:A:ASP:C | 1:54:A:THR:N | 1:54:A:THR:CA | 1:54:A:THR:C | 8 | 1.2 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 6 | 1.18 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 6 | 1.16 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 13 | 1.15 |
| (1,59) | 1:57:A:TYR:C | 1:58:A:GLU:N | 1:58:A:GLU:CA | 1:58:A:GLU:C | 9 | 1.15 |
| (1,116) | 1:100:A:MET:N | 1:100:A:MET:CA | 1:100:A:MET:C | 1:101:A:PHE:N | 3 | 1.14 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 3 | 1.12 |
| (1,67) | 1:61:A:VAL:C | 1:62:A:LEU:N | 1:62:A:LEU:CA | 1:62:A:LEU:C | 5 | 1.11 |
| (1,139) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:LEU:N | 23 | 1.1 |
| (1,116) | 1:100:A:MET:N | 1:100:A:MET:CA | 1:100:A:MET:C | 1:101:A:PHE:N | 18 | 1.1 |
| (1,173) | 1:57:A:TYR:N | 1:57:A:TYR:CA | 1:57:A:TYR:CB | 1:57:A:TYR:CG | 10 | 1.08 |
| (1,107) | 1:90:A:SER:C | 1:91:A:VAL:N | 1:91:A:VAL:CA | 1:91:A:VAL:C | 24 | 1.07 |
| (1,98) | 1:84:A:ASN:N | 1:84:A:ASN:CA | 1:84:A:ASN:C | 1:85:A:GLY:N | 9 | 1.04 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 16 | 1.03 |
| (1,83) | 1:76:A:LYS:C | 1:77:A:THR:N | 1:77:A:THR:CA | 1:77:A:THR:C | 16 | 1.02 |
| (1,41) | 1:46:A:LYS:C | 1:47:A:GLN:N | 1:47:A:GLN:CA | 1:47:A:GLN:C | 3 | 1.01 |