



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 09:38 AM UTC

PDB ID : 2MX1 / pdb_00002mx1
BMRB ID : 25381
Title : Structure of the E. coli Threonylcarbamoyl-AMP Synthase TSAC
Authors : Harris, K.A.; Bobay, B.G.; Sarachan, K.L.; Sims, A.F.; Bilbille, Y.; Deutsch, C.; Iwata-Reuyl, D.; Agris, P.F.
Deposited on : 2014-12-06

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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

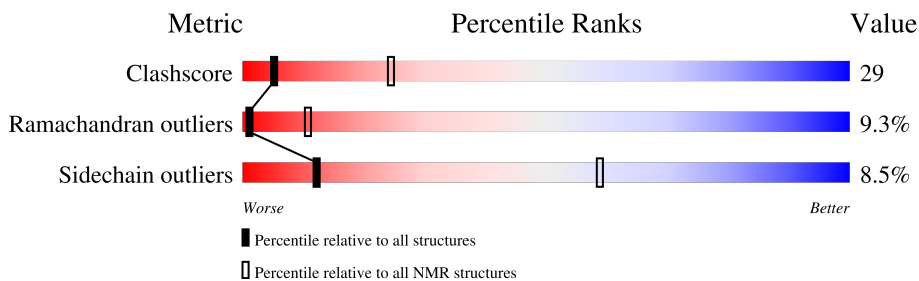
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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 | 229148 | 14424 |
| Ramachandran outliers | 224038 | 12848 |
| Sidechain outliers | 223484 | 12823 |

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 | 189 | |

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:4-A:101, A:105-A:169, A:177-A:184 (171) | 0.81 | 17 |

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2906 atoms, of which 1453 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Threonylcarbamoyl-AMP synthase.

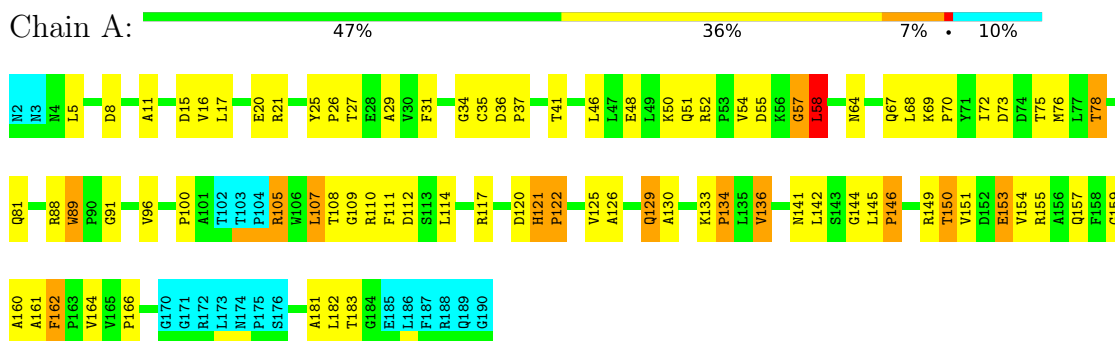
| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|-----|------|-----|-----|-------|---|
| | | | Total | C | H | N | O | | S |
| 1 | A | 189 | 2906 | 921 | 1453 | 253 | 274 | 5 | 0 |

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: Threonylcarbamoyl-AMP synthase

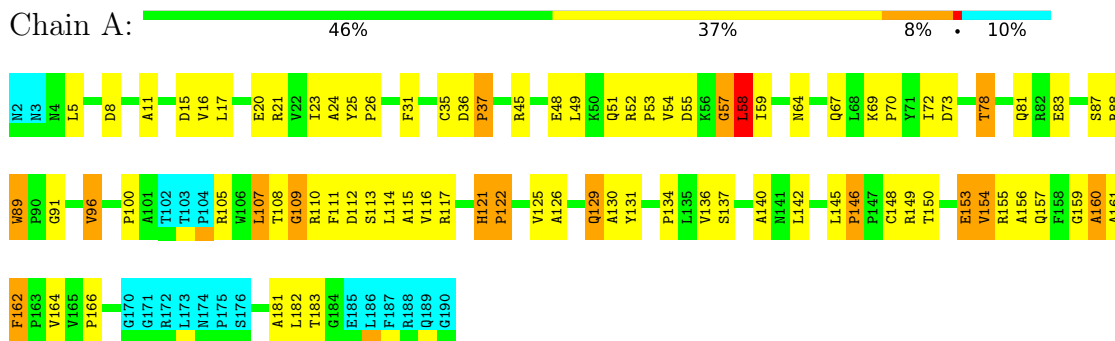


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

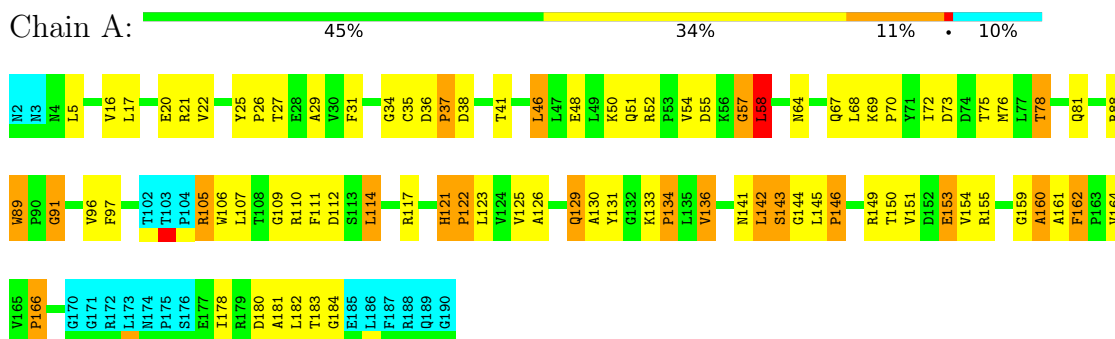
4.2.1 Score per residue for model 1

- Molecule 1: Threonylcarbamoyl-AMP synthase



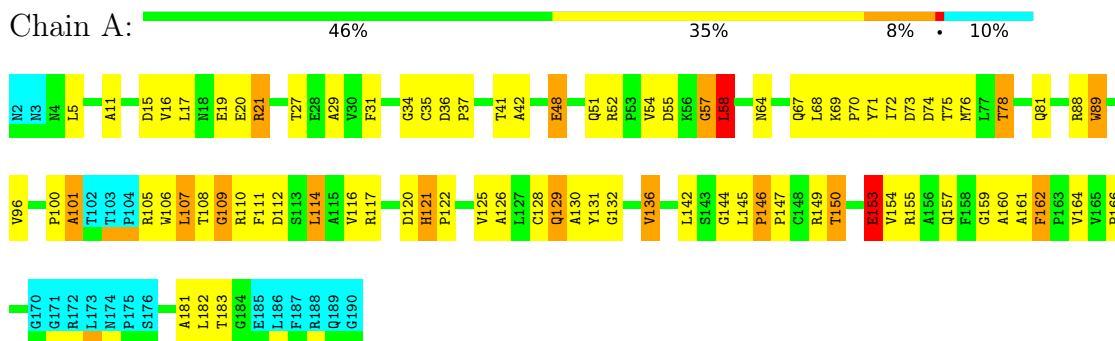
4.2.2 Score per residue for model 2

- Molecule 1: Threonylcarbamoyl-AMP synthase



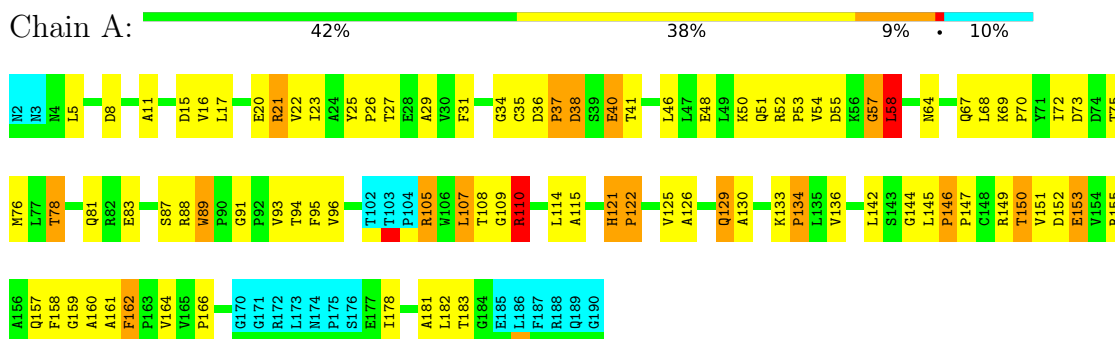
4.2.3 Score per residue for model 3

- Molecule 1: Threonylcarbamoyl-AMP synthase



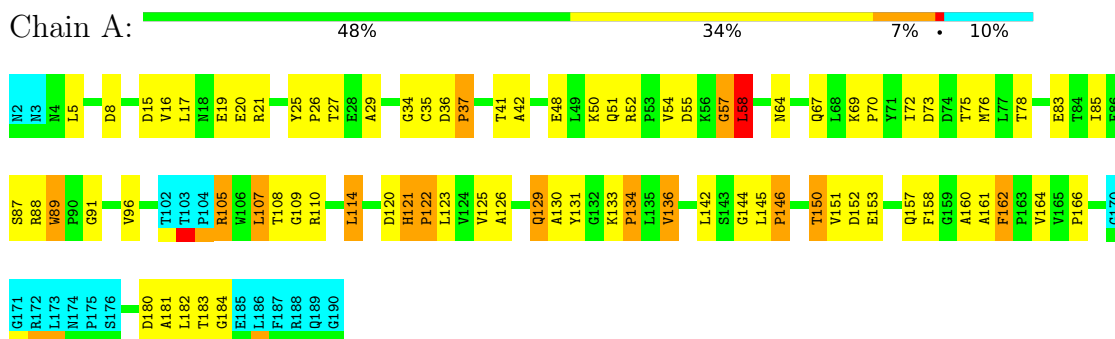
4.2.4 Score per residue for model 4

- Molecule 1: Threonylcarbamoyl-AMP synthase



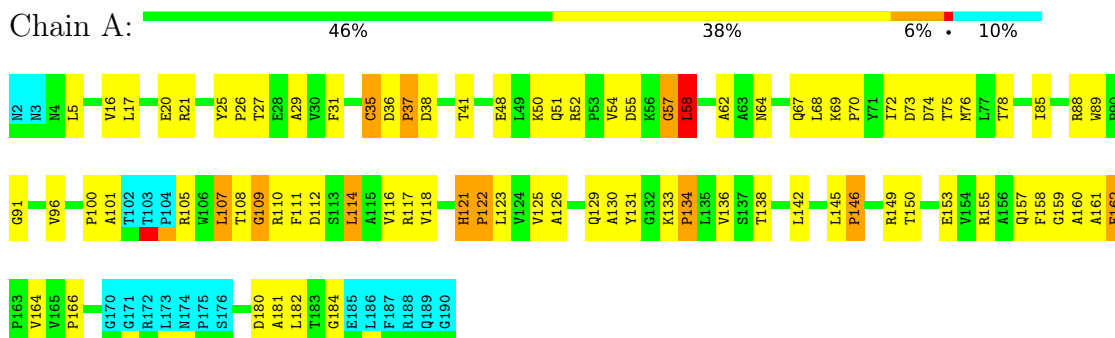
4.2.5 Score per residue for model 5

- Molecule 1: Threonylcarbamoyl-AMP synthase



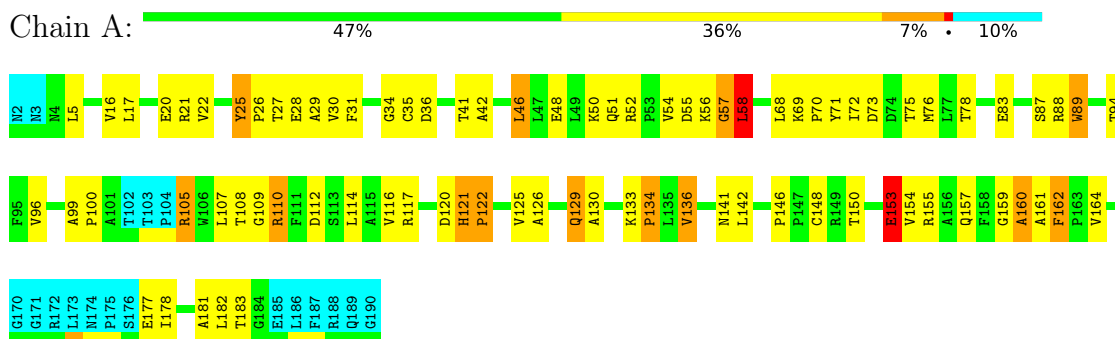
4.2.6 Score per residue for model 6

- Molecule 1: Threonylcarbamoyl-AMP synthase



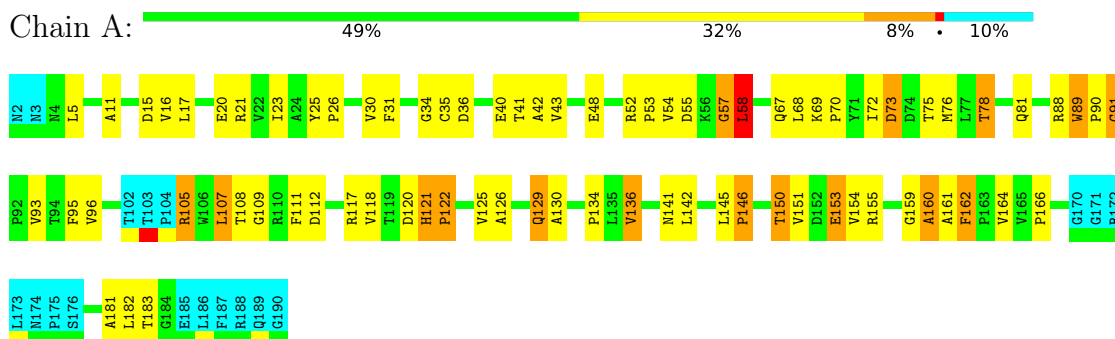
4.2.7 Score per residue for model 7

- Molecule 1: Threonylcarbamoyl-AMP synthase



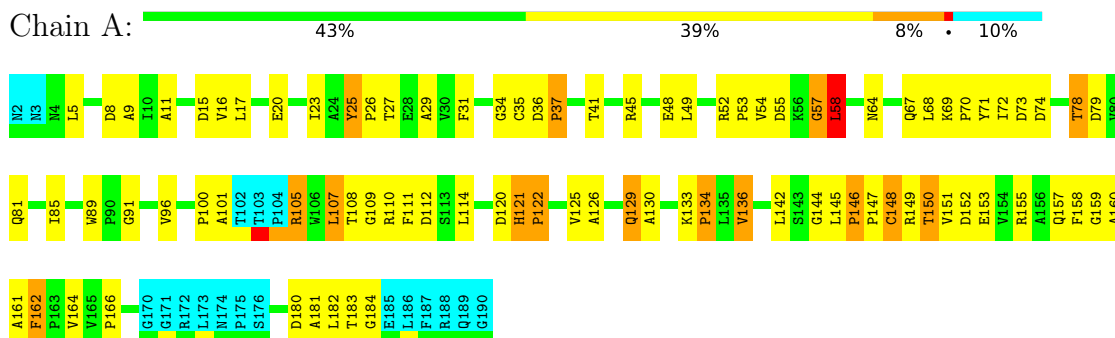
4.2.8 Score per residue for model 8

- Molecule 1: Threonylcarbamoyl-AMP synthase



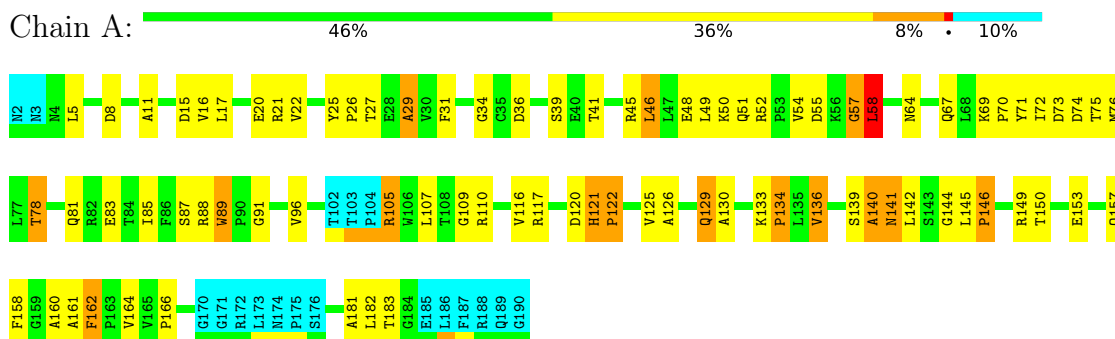
4.2.9 Score per residue for model 9

- Molecule 1: Threonylcarbamoyl-AMP synthase



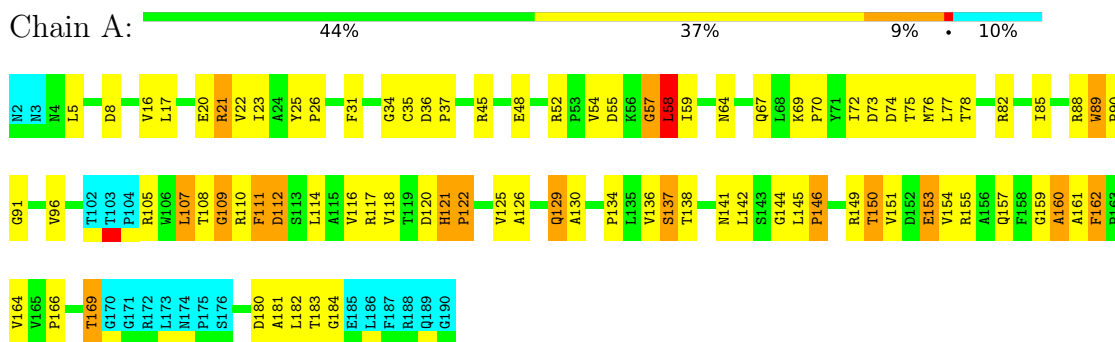
4.2.10 Score per residue for model 10

- Molecule 1: Threonylcarbamoyl-AMP synthase



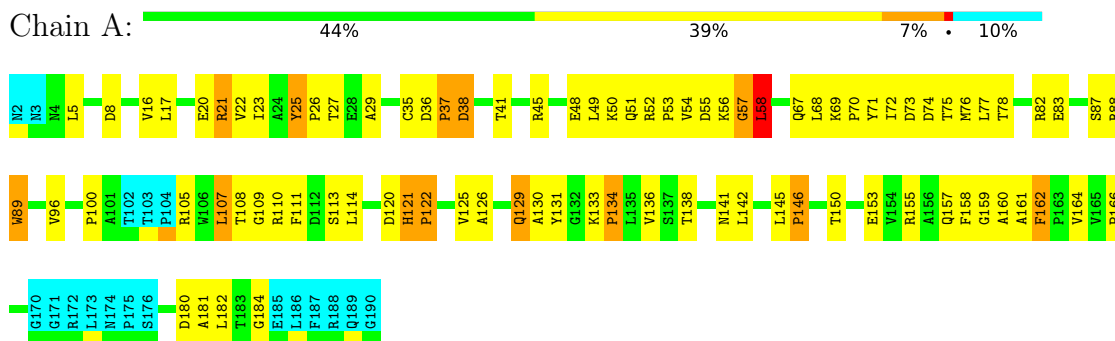
4.2.11 Score per residue for model 11

- Molecule 1: Threonylcarbamoyl-AMP synthase



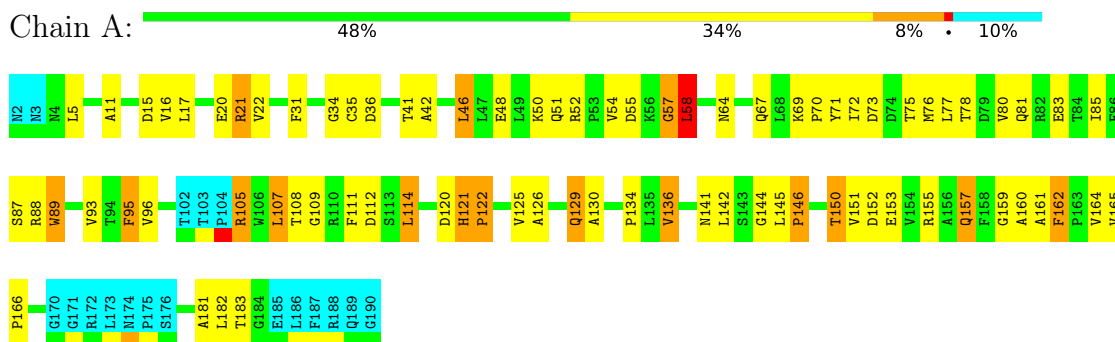
4.2.12 Score per residue for model 12

- Molecule 1: Threonylcarbamoyl-AMP synthase



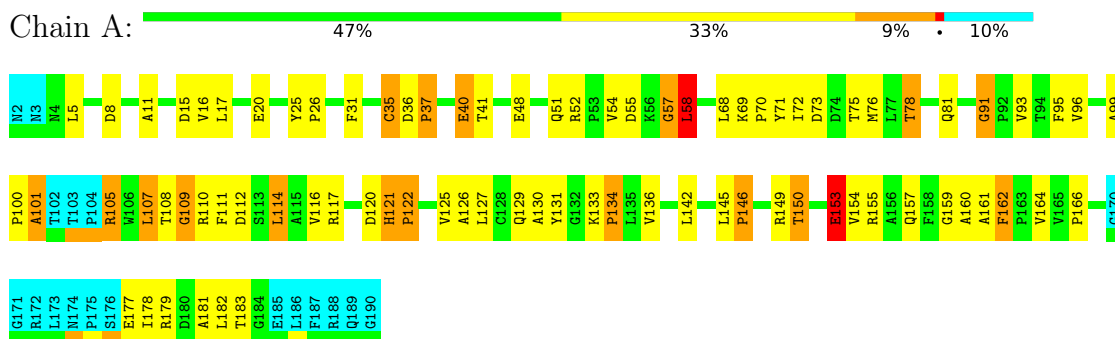
4.2.13 Score per residue for model 13

- Molecule 1: Threonylcarbamoyl-AMP synthase



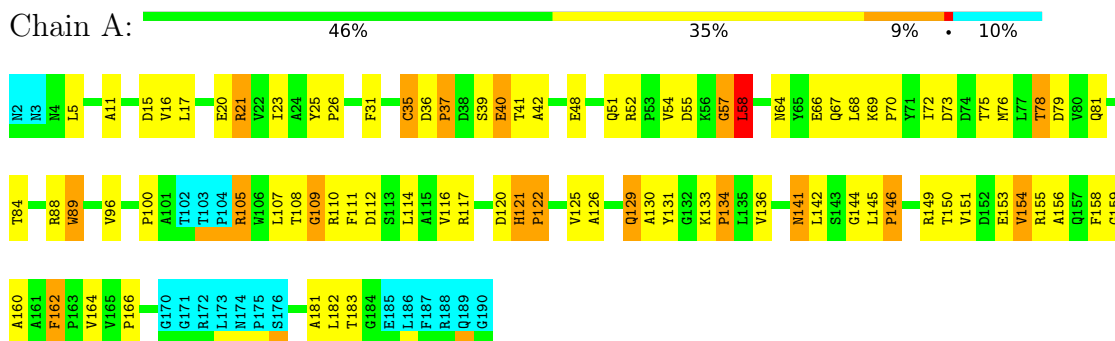
4.2.14 Score per residue for model 14

- Molecule 1: Threonylcarbamoyl-AMP synthase



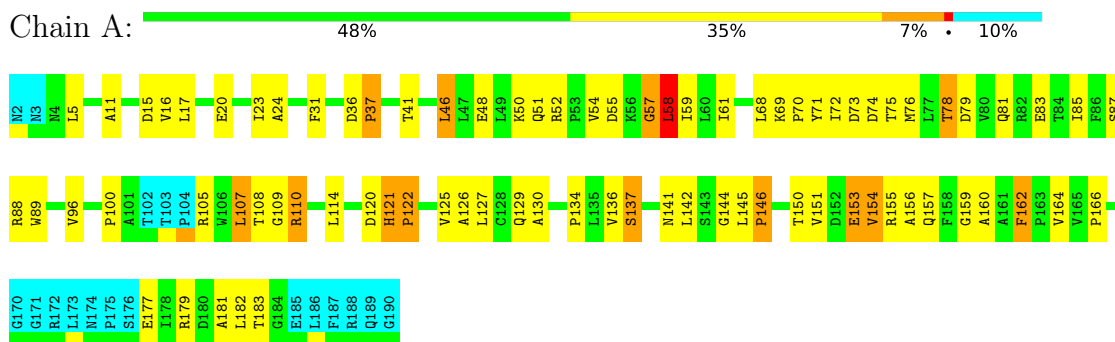
4.2.15 Score per residue for model 15

- Molecule 1: Threonylcarbamoyl-AMP synthase



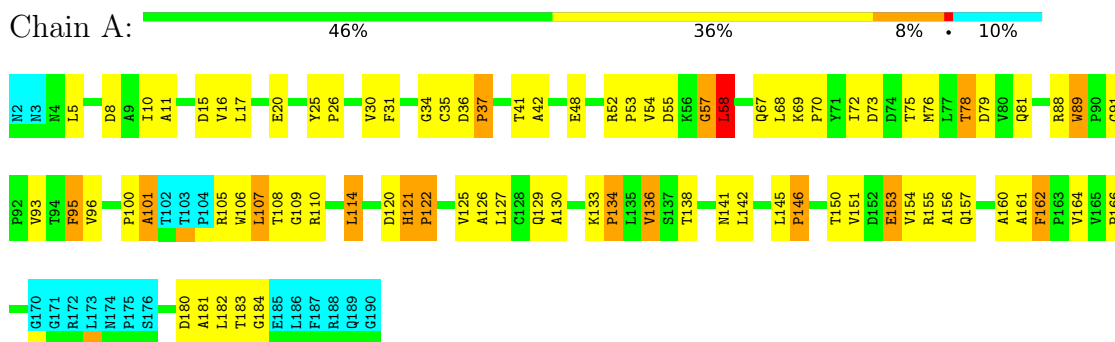
4.2.16 Score per residue for model 16

- Molecule 1: Threonylcarbamoyl-AMP synthase



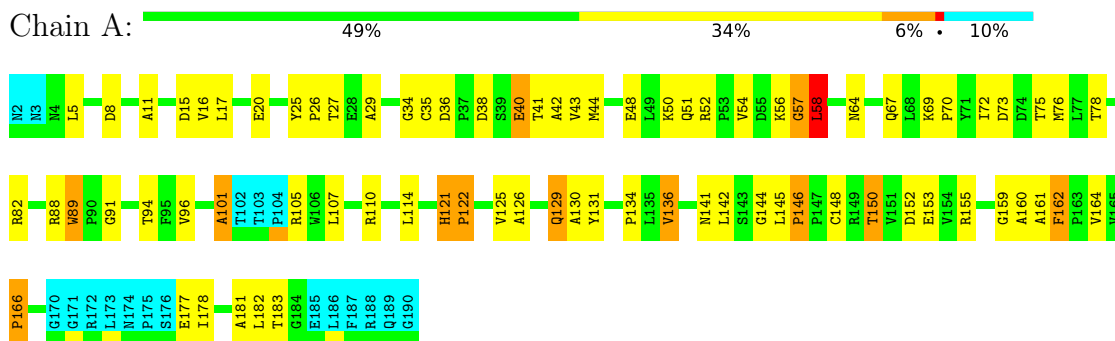
4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Threonylcarbamoyl-AMP synthase



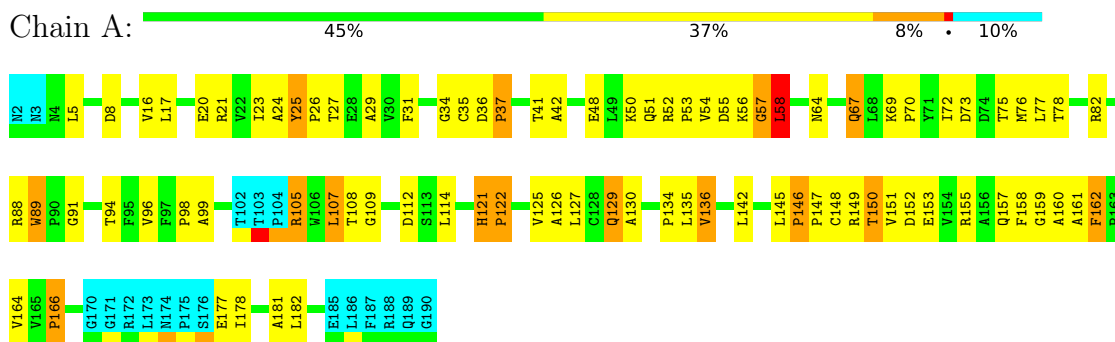
4.2.18 Score per residue for model 18

- Molecule 1: Threonylcarbamoyl-AMP synthase



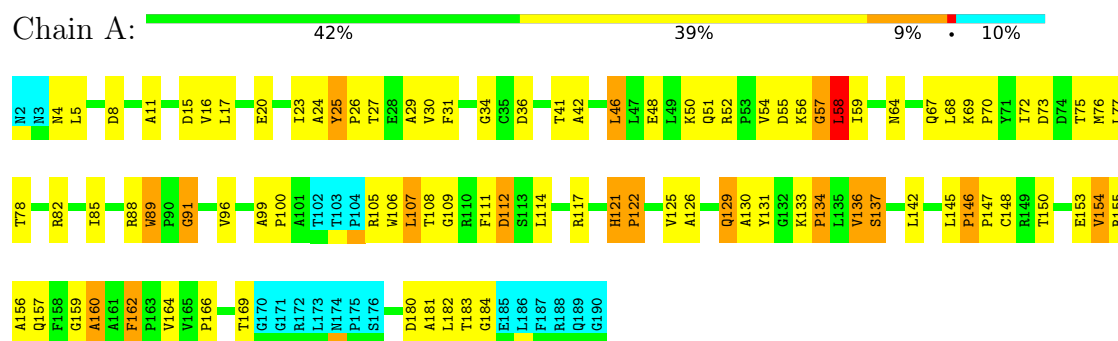
4.2.19 Score per residue for model 19

- Molecule 1: Threonylcarbamoyl-AMP synthase



4.2.20 Score per residue for model 20

- Molecule 1: Threonylcarbamoyl-AMP synthase



5 Refinement protocol and experimental data overview

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

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

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

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

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

| Chemical shift file(s) | working_cs.cif |
|--|----------------|
| Number of chemical shift lists | 1 |
| Total number of shifts | 1971 |
| Number of shifts mapped to atoms | 1971 |
| Number of unparsed shifts | 0 |
| Number of shifts with mapping errors | 0 |
| Number of shifts with mapping warnings | 0 |
| Assignment completeness (well-defined parts) | 78% |

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 1316 | 1322 | 1321 | 76±6 |
| All | All | 26320 | 26440 | 26420 | 1514 |

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 29.

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

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:107:LEU:H | 1:A:107:LEU:HD13 | 0.86 | 1.29 | 11 | 15 |
| 1:A:113:SER:C | 1:A:114:LEU:HD22 | 0.76 | 2.04 | 12 | 2 |
| 1:A:107:LEU:HD13 | 1:A:107:LEU:N | 0.73 | 1.99 | 16 | 15 |
| 1:A:96:VAL:O | 1:A:181:ALA:HB3 | 0.71 | 1.86 | 10 | 20 |
| 1:A:17:LEU:C | 1:A:17:LEU:HD23 | 0.67 | 2.14 | 17 | 19 |
| 1:A:142:LEU:C | 1:A:142:LEU:HD22 | 0.67 | 2.14 | 2 | 1 |
| 1:A:114:LEU:O | 1:A:114:LEU:HD12 | 0.67 | 1.90 | 16 | 7 |
| 1:A:127:LEU:C | 1:A:127:LEU:HD13 | 0.67 | 2.15 | 16 | 1 |
| 1:A:64:ASN:H | 1:A:67:GLN:NE2 | 0.65 | 1.90 | 11 | 13 |
| 1:A:107:LEU:H | 1:A:107:LEU:CD1 | 0.65 | 2.04 | 20 | 15 |
| 1:A:125:VAL:HG23 | 1:A:126:ALA:H | 0.65 | 1.51 | 13 | 20 |
| 1:A:17:LEU:C | 1:A:17:LEU:HD13 | 0.64 | 2.17 | 7 | 1 |
| 1:A:125:VAL:HG23 | 1:A:126:ALA:N | 0.64 | 2.08 | 3 | 20 |
| 1:A:111:PHE:CG | 1:A:112:ASP:N | 0.61 | 2.67 | 15 | 7 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:107:LEU:HD22 | 1:A:108:THR:H | 0.60 | 1.54 | 11 | 14 |
| 1:A:95:PHE:CD1 | 1:A:95:PHE:N | 0.60 | 2.70 | 13 | 2 |
| 1:A:75:THR:HG23 | 1:A:76:MET:N | 0.60 | 2.12 | 5 | 16 |
| 1:A:5:LEU:HD22 | 1:A:5:LEU:N | 0.59 | 2.11 | 19 | 1 |
| 1:A:121:HIS:H | 1:A:122:PRO:CD | 0.59 | 2.11 | 20 | 20 |
| 1:A:142:LEU:N | 1:A:142:LEU:HD13 | 0.59 | 2.13 | 2 | 1 |
| 1:A:72:ILE:HG22 | 1:A:73:ASP:N | 0.58 | 2.14 | 18 | 20 |
| 1:A:111:PHE:CD2 | 1:A:112:ASP:N | 0.57 | 2.72 | 3 | 4 |
| 1:A:107:LEU:H | 1:A:107:LEU:CD2 | 0.57 | 2.12 | 18 | 5 |
| 1:A:58:LEU:N | 1:A:58:LEU:CD2 | 0.57 | 2.67 | 1 | 20 |
| 1:A:88:ARG:O | 1:A:89:TRP:CG | 0.57 | 2.58 | 16 | 2 |
| 1:A:100:PRO:O | 1:A:101:ALA:HB3 | 0.57 | 2.00 | 14 | 3 |
| 1:A:40:GLU:CD | 1:A:40:GLU:H | 0.56 | 2.08 | 4 | 4 |
| 1:A:35:CYS:SG | 1:A:36:ASP:N | 0.56 | 2.78 | 15 | 17 |
| 1:A:142:LEU:N | 1:A:142:LEU:CD1 | 0.56 | 2.68 | 2 | 1 |
| 1:A:54:VAL:HG13 | 1:A:55:ASP:N | 0.56 | 2.16 | 19 | 19 |
| 1:A:107:LEU:HD22 | 1:A:108:THR:N | 0.56 | 2.16 | 16 | 14 |
| 1:A:55:ASP:OD1 | 1:A:110:ARG:N | 0.56 | 2.39 | 11 | 6 |
| 1:A:108:THR:O | 1:A:110:ARG:N | 0.56 | 2.39 | 3 | 6 |
| 1:A:108:THR:OG1 | 1:A:114:LEU:HD11 | 0.55 | 2.00 | 12 | 1 |
| 1:A:89:TRP:N | 1:A:89:TRP:CD1 | 0.55 | 2.69 | 19 | 1 |
| 1:A:46:LEU:C | 1:A:46:LEU:HD13 | 0.55 | 2.26 | 4 | 1 |
| 1:A:108:THR:OG1 | 1:A:114:LEU:HD21 | 0.55 | 2.02 | 11 | 1 |
| 1:A:106:TRP:CD1 | 1:A:106:TRP:N | 0.55 | 2.72 | 20 | 2 |
| 1:A:177:GLU:H | 1:A:179:ARG:NH1 | 0.55 | 2.00 | 16 | 1 |
| 1:A:126:ALA:O | 1:A:130:ALA:HB2 | 0.54 | 2.03 | 5 | 19 |
| 1:A:142:LEU:HD13 | 1:A:142:LEU:H | 0.54 | 1.62 | 2 | 1 |
| 1:A:25:TYR:CE2 | 1:A:26:PRO:O | 0.54 | 2.60 | 6 | 5 |
| 1:A:120:ASP:O | 1:A:121:HIS:CG | 0.54 | 2.60 | 3 | 1 |
| 1:A:36:ASP:CG | 1:A:131:TYR:CZ | 0.54 | 2.86 | 1 | 4 |
| 1:A:155:ARG:O | 1:A:159:GLY:N | 0.54 | 2.41 | 15 | 15 |
| 1:A:25:TYR:CE1 | 1:A:26:PRO:O | 0.54 | 2.61 | 8 | 10 |
| 1:A:105:ARG:O | 1:A:109:GLY:N | 0.54 | 2.41 | 7 | 19 |
| 1:A:111:PHE:CE2 | 1:A:112:ASP:OD1 | 0.53 | 2.61 | 14 | 2 |
| 1:A:31:PHE:CD1 | 1:A:149:ARG:O | 0.53 | 2.61 | 15 | 1 |
| 1:A:25:TYR:CZ | 1:A:26:PRO:O | 0.53 | 2.61 | 19 | 10 |
| 1:A:153:GLU:O | 1:A:155:ARG:N | 0.53 | 2.41 | 1 | 9 |
| 1:A:93:VAL:O | 1:A:95:PHE:CE1 | 0.53 | 2.61 | 17 | 2 |
| 1:A:31:PHE:CD2 | 1:A:149:ARG:O | 0.53 | 2.62 | 11 | 8 |
| 1:A:153:GLU:OE1 | 1:A:157:GLN:NE2 | 0.53 | 2.42 | 6 | 2 |
| 1:A:91:GLY:O | 1:A:117:ARG:NE | 0.53 | 2.42 | 20 | 4 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:105:ARG:NH2 | 1:A:110:ARG:O | 0.53 | 2.42 | 16 | 5 |
| 1:A:31:PHE:CD2 | 1:A:148:CYS:O | 0.53 | 2.62 | 20 | 2 |
| 1:A:111:PHE:CE1 | 1:A:112:ASP:OD1 | 0.52 | 2.62 | 1 | 1 |
| 1:A:68:LEU:N | 1:A:68:LEU:HD22 | 0.52 | 2.18 | 17 | 13 |
| 1:A:71:TYR:O | 1:A:71:TYR:CD1 | 0.52 | 2.62 | 10 | 4 |
| 1:A:94:THR:N | 1:A:177:GLU:O | 0.52 | 2.42 | 19 | 3 |
| 1:A:76:MET:HE1 | 1:A:181:ALA:O | 0.52 | 2.04 | 11 | 1 |
| 1:A:8:ASP:OD1 | 1:A:9:ALA:N | 0.52 | 2.42 | 9 | 1 |
| 1:A:180:ASP:O | 1:A:184:GLY:N | 0.52 | 2.41 | 12 | 8 |
| 1:A:41:THR:HG23 | 1:A:42:ALA:N | 0.52 | 2.17 | 5 | 9 |
| 1:A:147:PRO:O | 1:A:149:ARG:N | 0.52 | 2.42 | 9 | 2 |
| 1:A:183:THR:HG23 | 1:A:184:GLY:N | 0.52 | 2.19 | 9 | 2 |
| 1:A:36:ASP:OD1 | 1:A:36:ASP:N | 0.52 | 2.42 | 17 | 1 |
| 1:A:121:HIS:N | 1:A:122:PRO:CD | 0.52 | 2.73 | 2 | 20 |
| 1:A:177:GLU:CD | 1:A:178:ILE:N | 0.52 | 2.67 | 18 | 1 |
| 1:A:84:THR:O | 1:A:88:ARG:N | 0.52 | 2.42 | 15 | 1 |
| 1:A:161:ALA:O | 1:A:162:PHE:CD2 | 0.52 | 2.62 | 7 | 17 |
| 1:A:96:VAL:HG13 | 1:A:114:LEU:C | 0.52 | 2.30 | 4 | 15 |
| 1:A:83:GLU:O | 1:A:87:SER:N | 0.52 | 2.43 | 16 | 8 |
| 1:A:93:VAL:CG1 | 1:A:95:PHE:CZ | 0.52 | 2.93 | 14 | 1 |
| 1:A:111:PHE:CZ | 1:A:112:ASP:OD1 | 0.51 | 2.63 | 1 | 1 |
| 1:A:108:THR:C | 1:A:110:ARG:H | 0.51 | 2.13 | 3 | 6 |
| 1:A:36:ASP:OD1 | 1:A:131:TYR:CE1 | 0.51 | 2.63 | 6 | 2 |
| 1:A:31:PHE:CD1 | 1:A:148:CYS:O | 0.51 | 2.63 | 9 | 2 |
| 1:A:5:LEU:N | 1:A:5:LEU:HD12 | 0.51 | 2.21 | 13 | 19 |
| 1:A:91:GLY:O | 1:A:117:ARG:NH2 | 0.51 | 2.43 | 20 | 3 |
| 1:A:107:LEU:H | 1:A:107:LEU:HD23 | 0.51 | 1.65 | 7 | 4 |
| 1:A:58:LEU:N | 1:A:58:LEU:HD23 | 0.51 | 2.21 | 10 | 20 |
| 1:A:120:ASP:O | 1:A:121:HIS:ND1 | 0.50 | 2.43 | 3 | 1 |
| 1:A:177:GLU:OE1 | 1:A:179:ARG:NH1 | 0.50 | 2.43 | 14 | 1 |
| 1:A:148:CYS:SG | 1:A:148:CYS:O | 0.50 | 2.69 | 1 | 2 |
| 1:A:153:GLU:O | 1:A:156:ALA:N | 0.50 | 2.44 | 1 | 5 |
| 1:A:107:LEU:HD23 | 1:A:107:LEU:N | 0.50 | 2.21 | 7 | 5 |
| 1:A:31:PHE:CE2 | 1:A:149:ARG:O | 0.50 | 2.65 | 2 | 2 |
| 1:A:100:PRO:O | 1:A:101:ALA:CB | 0.50 | 2.60 | 3 | 3 |
| 1:A:17:LEU:C | 1:A:17:LEU:CD2 | 0.50 | 2.85 | 10 | 19 |
| 1:A:36:ASP:OD2 | 1:A:131:TYR:CE1 | 0.50 | 2.65 | 12 | 5 |
| 1:A:93:VAL:CG1 | 1:A:95:PHE:CE2 | 0.50 | 2.95 | 14 | 1 |
| 1:A:125:VAL:CG2 | 1:A:126:ALA:N | 0.50 | 2.75 | 3 | 20 |
| 1:A:182:LEU:CD2 | 1:A:182:LEU:N | 0.50 | 2.75 | 6 | 20 |
| 1:A:107:LEU:N | 1:A:107:LEU:CD1 | 0.50 | 2.74 | 13 | 12 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:140:ALA:HB1 | 1:A:148:CYS:SG | 0.50 | 2.46 | 1 | 1 |
| 1:A:72:ILE:CG2 | 1:A:73:ASP:N | 0.49 | 2.76 | 3 | 16 |
| 1:A:16:VAL:O | 1:A:20:GLU:N | 0.49 | 2.42 | 15 | 20 |
| 1:A:105:ARG:NH1 | 1:A:112:ASP:OD1 | 0.49 | 2.45 | 15 | 2 |
| 1:A:71:TYR:OH | 1:A:114:LEU:HD21 | 0.49 | 2.07 | 14 | 3 |
| 1:A:129:GLN:CD | 1:A:129:GLN:C | 0.49 | 2.80 | 17 | 20 |
| 1:A:116:VAL:HG22 | 1:A:117:ARG:N | 0.49 | 2.22 | 6 | 8 |
| 1:A:99:ALA:N | 1:A:112:ASP:O | 0.49 | 2.45 | 14 | 2 |
| 1:A:54:VAL:CG1 | 1:A:55:ASP:N | 0.49 | 2.76 | 11 | 12 |
| 1:A:105:ARG:NH1 | 1:A:110:ARG:O | 0.49 | 2.45 | 5 | 1 |
| 1:A:75:THR:OG1 | 1:A:76:MET:N | 0.48 | 2.46 | 8 | 1 |
| 1:A:77:LEU:HD21 | 1:A:82:ARG:NH2 | 0.48 | 2.22 | 12 | 3 |
| 1:A:35:CYS:O | 1:A:135:LEU:HD12 | 0.48 | 2.07 | 19 | 1 |
| 1:A:88:ARG:O | 1:A:89:TRP:CD1 | 0.48 | 2.67 | 6 | 1 |
| 1:A:56:LYS:CD | 1:A:56:LYS:N | 0.48 | 2.76 | 12 | 4 |
| 1:A:108:THR:C | 1:A:110:ARG:N | 0.48 | 2.71 | 3 | 6 |
| 1:A:142:LEU:C | 1:A:142:LEU:CD2 | 0.48 | 2.86 | 2 | 1 |
| 1:A:69:LYS:N | 1:A:70:PRO:CD | 0.48 | 2.77 | 12 | 20 |
| 1:A:142:LEU:O | 1:A:144:GLY:N | 0.48 | 2.47 | 2 | 1 |
| 1:A:114:LEU:HD12 | 1:A:114:LEU:C | 0.48 | 2.33 | 16 | 1 |
| 1:A:128:CYS:O | 1:A:132:GLY:N | 0.48 | 2.47 | 3 | 1 |
| 1:A:78:THR:OG1 | 1:A:79:ASP:N | 0.48 | 2.46 | 16 | 1 |
| 1:A:5:LEU:N | 1:A:5:LEU:CD2 | 0.48 | 2.77 | 19 | 1 |
| 1:A:22:VAL:HG23 | 1:A:34:GLY:O | 0.47 | 2.09 | 13 | 5 |
| 1:A:16:VAL:HG13 | 1:A:21:ARG:O | 0.47 | 2.09 | 11 | 5 |
| 1:A:157:GLN:CG | 1:A:158:PHE:N | 0.47 | 2.76 | 5 | 7 |
| 1:A:40:GLU:O | 1:A:43:VAL:HG12 | 0.47 | 2.09 | 8 | 1 |
| 1:A:78:THR:O | 1:A:81:GLN:N | 0.47 | 2.47 | 15 | 10 |
| 1:A:145:LEU:C | 1:A:145:LEU:HD13 | 0.47 | 2.34 | 16 | 3 |
| 1:A:125:VAL:O | 1:A:129:GLN:N | 0.47 | 2.40 | 20 | 20 |
| 1:A:153:GLU:C | 1:A:155:ARG:N | 0.47 | 2.71 | 1 | 7 |
| 1:A:69:LYS:NZ | 1:A:82:ARG:HH12 | 0.47 | 2.08 | 18 | 1 |
| 1:A:91:GLY:O | 1:A:117:ARG:CZ | 0.47 | 2.62 | 20 | 1 |
| 1:A:125:VAL:CG2 | 1:A:126:ALA:H | 0.47 | 2.21 | 20 | 20 |
| 1:A:162:PHE:C | 1:A:164:VAL:H | 0.47 | 2.18 | 16 | 20 |
| 1:A:68:LEU:N | 1:A:68:LEU:CD2 | 0.47 | 2.78 | 17 | 7 |
| 1:A:36:ASP:O | 1:A:37:PRO:O | 0.47 | 2.32 | 14 | 12 |
| 1:A:68:LEU:O | 1:A:72:ILE:HD13 | 0.47 | 2.09 | 3 | 3 |
| 1:A:182:LEU:N | 1:A:182:LEU:HD22 | 0.47 | 2.24 | 5 | 19 |
| 1:A:28:GLU:OE2 | 1:A:117:ARG:NH1 | 0.47 | 2.47 | 7 | 1 |
| 1:A:162:PHE:C | 1:A:162:PHE:CD1 | 0.47 | 2.90 | 15 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:31:PHE:CZ | 1:A:151:VAL:HG13 | 0.47 | 2.45 | 16 | 1 |
| 1:A:5:LEU:N | 1:A:5:LEU:CD1 | 0.47 | 2.78 | 13 | 16 |
| 1:A:35:CYS:SG | 1:A:42:ALA:HB2 | 0.47 | 2.50 | 8 | 3 |
| 1:A:157:GLN:HE21 | 1:A:157:GLN:C | 0.47 | 2.17 | 13 | 1 |
| 1:A:73:ASP:C | 1:A:75:THR:N | 0.46 | 2.72 | 13 | 2 |
| 1:A:31:PHE:CE1 | 1:A:149:ARG:O | 0.46 | 2.68 | 15 | 1 |
| 1:A:71:TYR:OH | 1:A:114:LEU:CD2 | 0.46 | 2.63 | 3 | 3 |
| 1:A:75:THR:HG23 | 1:A:76:MET:H | 0.46 | 1.69 | 5 | 1 |
| 1:A:75:THR:CG2 | 1:A:76:MET:N | 0.46 | 2.78 | 5 | 10 |
| 1:A:88:ARG:O | 1:A:89:TRP:C | 0.46 | 2.59 | 3 | 4 |
| 1:A:107:LEU:CD2 | 1:A:107:LEU:N | 0.46 | 2.78 | 10 | 5 |
| 1:A:142:LEU:O | 1:A:143:SER:C | 0.46 | 2.59 | 2 | 1 |
| 1:A:19:GLU:O | 1:A:21:ARG:NH1 | 0.46 | 2.49 | 3 | 1 |
| 1:A:41:THR:CG2 | 1:A:42:ALA:N | 0.46 | 2.79 | 5 | 6 |
| 1:A:125:VAL:O | 1:A:126:ALA:C | 0.46 | 2.59 | 1 | 20 |
| 1:A:85:ILE:O | 1:A:89:TRP:O | 0.46 | 2.34 | 16 | 7 |
| 1:A:105:ARG:O | 1:A:109:GLY:CA | 0.46 | 2.64 | 20 | 1 |
| 1:A:123:LEU:HD12 | 1:A:123:LEU:N | 0.46 | 2.26 | 2 | 3 |
| 1:A:111:PHE:CD2 | 1:A:112:ASP:OD1 | 0.45 | 2.70 | 14 | 1 |
| 1:A:141:ASN:ND2 | 1:A:141:ASN:C | 0.45 | 2.71 | 15 | 1 |
| 1:A:88:ARG:O | 1:A:89:TRP:O | 0.45 | 2.34 | 2 | 13 |
| 1:A:69:LYS:CB | 1:A:69:LYS:NZ | 0.45 | 2.79 | 11 | 1 |
| 1:A:45:ARG:O | 1:A:49:LEU:CD2 | 0.45 | 2.65 | 9 | 3 |
| 1:A:105:ARG:CZ | 1:A:110:ARG:O | 0.45 | 2.64 | 10 | 1 |
| 1:A:140:ALA:O | 1:A:141:ASN:CG | 0.45 | 2.60 | 10 | 1 |
| 1:A:27:THR:C | 1:A:29:ALA:H | 0.45 | 2.20 | 4 | 12 |
| 1:A:141:ASN:ND2 | 1:A:141:ASN:O | 0.45 | 2.49 | 15 | 1 |
| 1:A:59:ILE:O | 1:A:137:SER:OG | 0.45 | 2.35 | 16 | 4 |
| 1:A:55:ASP:OD1 | 1:A:108:THR:O | 0.45 | 2.35 | 1 | 5 |
| 1:A:62:ALA:HB3 | 1:A:118:VAL:HG22 | 0.45 | 1.89 | 6 | 1 |
| 1:A:77:LEU:HD11 | 1:A:82:ARG:NE | 0.45 | 2.25 | 20 | 1 |
| 1:A:23:ILE:HD12 | 1:A:23:ILE:C | 0.45 | 2.37 | 1 | 5 |
| 1:A:57:GLY:O | 1:A:58:LEU:O | 0.45 | 2.35 | 20 | 20 |
| 1:A:71:TYR:OH | 1:A:114:LEU:CD1 | 0.45 | 2.65 | 9 | 1 |
| 1:A:55:ASP:O | 1:A:108:THR:O | 0.45 | 2.35 | 3 | 5 |
| 1:A:80:VAL:HG13 | 1:A:81:GLN:N | 0.45 | 2.27 | 13 | 1 |
| 1:A:8:ASP:OD1 | 1:A:8:ASP:C | 0.44 | 2.61 | 19 | 7 |
| 1:A:153:GLU:OE1 | 1:A:157:GLN:OE1 | 0.44 | 2.36 | 12 | 5 |
| 1:A:17:LEU:C | 1:A:17:LEU:CD1 | 0.44 | 2.88 | 7 | 1 |
| 1:A:73:ASP:C | 1:A:75:THR:H | 0.44 | 2.18 | 13 | 1 |
| 1:A:178:ILE:HG23 | 1:A:178:ILE:O | 0.44 | 2.12 | 2 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:45:ARG:NH2 | 1:A:138:THR:OG1 | 0.44 | 2.50 | 11 | 1 |
| 1:A:50:LYS:O | 1:A:51:GLN:C | 0.44 | 2.60 | 18 | 12 |
| 1:A:150:THR:O | 1:A:153:GLU:N | 0.44 | 2.49 | 9 | 8 |
| 1:A:120:ASP:O | 1:A:120:ASP:OD1 | 0.44 | 2.36 | 11 | 10 |
| 1:A:11:ALA:O | 1:A:15:ASP:CG | 0.44 | 2.61 | 17 | 13 |
| 1:A:164:VAL:HG23 | 1:A:166:PRO:HD3 | 0.44 | 1.89 | 6 | 18 |
| 1:A:90:PRO:O | 1:A:118:VAL:O | 0.44 | 2.36 | 8 | 2 |
| 1:A:94:THR:O | 1:A:177:GLU:O | 0.44 | 2.36 | 19 | 1 |
| 1:A:55:ASP:OD1 | 1:A:110:ARG:CA | 0.44 | 2.65 | 3 | 2 |
| 1:A:100:PRO:O | 1:A:101:ALA:O | 0.44 | 2.36 | 17 | 1 |
| 1:A:129:GLN:C | 1:A:129:GLN:NE2 | 0.44 | 2.76 | 7 | 2 |
| 1:A:55:ASP:O | 1:A:55:ASP:OD1 | 0.44 | 2.36 | 12 | 3 |
| 1:A:8:ASP:OD1 | 1:A:162:PHE:O | 0.44 | 2.36 | 19 | 6 |
| 1:A:133:LYS:O | 1:A:134:PRO:O | 0.44 | 2.36 | 9 | 12 |
| 1:A:139:SER:O | 1:A:140:ALA:O | 0.44 | 2.36 | 10 | 1 |
| 1:A:53:PRO:O | 1:A:54:VAL:C | 0.43 | 2.62 | 12 | 7 |
| 1:A:145:LEU:O | 1:A:146:PRO:C | 0.43 | 2.61 | 16 | 19 |
| 1:A:141:ASN:OD1 | 1:A:141:ASN:O | 0.43 | 2.37 | 2 | 3 |
| 1:A:147:PRO:O | 1:A:153:GLU:OE2 | 0.43 | 2.36 | 3 | 1 |
| 1:A:5:LEU:CD2 | 1:A:5:LEU:H | 0.43 | 2.26 | 19 | 1 |
| 1:A:85:ILE:O | 1:A:88:ARG:O | 0.43 | 2.36 | 13 | 1 |
| 1:A:59:ILE:O | 1:A:137:SER:CB | 0.43 | 2.66 | 16 | 2 |
| 1:A:8:ASP:OD2 | 1:A:164:VAL:O | 0.43 | 2.37 | 17 | 2 |
| 1:A:112:ASP:OD1 | 1:A:112:ASP:O | 0.43 | 2.36 | 6 | 1 |
| 1:A:145:LEU:O | 1:A:146:PRO:O | 0.43 | 2.37 | 6 | 4 |
| 1:A:77:LEU:CD1 | 1:A:77:LEU:N | 0.43 | 2.80 | 13 | 1 |
| 1:A:84:THR:O | 1:A:88:ARG:CB | 0.43 | 2.66 | 15 | 1 |
| 1:A:17:LEU:HD23 | 1:A:17:LEU:O | 0.43 | 2.14 | 4 | 14 |
| 1:A:36:ASP:CG | 1:A:131:TYR:OH | 0.43 | 2.62 | 20 | 2 |
| 1:A:140:ALA:O | 1:A:141:ASN:O | 0.43 | 2.36 | 10 | 1 |
| 1:A:157:GLN:O | 1:A:157:GLN:NE2 | 0.43 | 2.50 | 13 | 1 |
| 1:A:127:LEU:C | 1:A:127:LEU:CD1 | 0.43 | 2.86 | 16 | 1 |
| 1:A:37:PRO:O | 1:A:38:ASP:C | 0.43 | 2.62 | 12 | 3 |
| 1:A:21:ARG:NH2 | 1:A:22:VAL:O | 0.43 | 2.50 | 4 | 3 |
| 1:A:36:ASP:N | 1:A:36:ASP:OD1 | 0.43 | 2.45 | 4 | 2 |
| 1:A:93:VAL:HG13 | 1:A:95:PHE:CE2 | 0.43 | 2.48 | 8 | 2 |
| 1:A:178:ILE:O | 1:A:178:ILE:HG23 | 0.43 | 2.13 | 18 | 4 |
| 1:A:73:ASP:O | 1:A:74:ASP:CG | 0.43 | 2.62 | 10 | 1 |
| 1:A:36:ASP:OD2 | 1:A:131:TYR:CD1 | 0.43 | 2.71 | 14 | 1 |
| 1:A:55:ASP:OD1 | 1:A:109:GLY:C | 0.43 | 2.62 | 1 | 2 |
| 1:A:36:ASP:O | 1:A:37:PRO:C | 0.43 | 2.61 | 11 | 2 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|-----------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:141:ASN:C | 1:A:141:ASN:HD22 | 0.43 | 2.20 | 15 | 1 |
| 1:A:69:LYS:NZ | 1:A:82:ARG:NH1 | 0.43 | 2.67 | 18 | 1 |
| 1:A:96:VAL:HG13 | 1:A:115:ALA:N | 0.43 | 2.28 | 1 | 1 |
| 1:A:129:GLN:HG3 | 1:A:130:ALA:N | 0.43 | 2.28 | 6 | 19 |
| 1:A:54:VAL:O | 1:A:108:THR:O | 0.43 | 2.37 | 7 | 3 |
| 1:A:112:ASP:OD1 | 1:A:112:ASP:C | 0.43 | 2.62 | 6 | 3 |
| 1:A:141:ASN:OD1 | 1:A:141:ASN:C | 0.43 | 2.62 | 8 | 5 |
| 1:A:36:ASP:CG | 1:A:39:SER:OG | 0.43 | 2.62 | 10 | 1 |
| 1:A:74:ASP:O | 1:A:74:ASP:OD1 | 0.43 | 2.37 | 9 | 4 |
| 1:A:8:ASP:C | 1:A:8:ASP:OD1 | 0.43 | 2.62 | 5 | 3 |
| 1:A:106:TRP:C | 1:A:106:TRP:CD1 | 0.43 | 2.96 | 2 | 1 |
| 1:A:157:GLN:C | 1:A:157:GLN:NE2 | 0.43 | 2.77 | 13 | 1 |
| 1:A:10:ILE:CG2 | 1:A:11:ALA:N | 0.43 | 2.82 | 17 | 1 |
| 1:A:116:VAL:CG2 | 1:A:117:ARG:N | 0.42 | 2.81 | 6 | 2 |
| 1:A:55:ASP:OD1 | 1:A:55:ASP:C | 0.42 | 2.62 | 17 | 7 |
| 1:A:30:VAL:O | 1:A:31:PHE:C | 0.42 | 2.62 | 8 | 4 |
| 1:A:64:ASN:O | 1:A:67:GLN:CD | 0.42 | 2.61 | 15 | 2 |
| 1:A:61:ILE:O | 1:A:61:ILE:HG23 | 0.42 | 2.13 | 16 | 1 |
| 1:A:51:GLN:O | 1:A:51:GLN:CG | 0.42 | 2.68 | 3 | 4 |
| 1:A:159:GLY:O | 1:A:160:ALA:O | 0.42 | 2.37 | 2 | 6 |
| 1:A:105:ARG:NE | 1:A:110:ARG:O | 0.42 | 2.52 | 4 | 1 |
| 1:A:147:PRO:O | 1:A:153:GLU:OE1 | 0.42 | 2.37 | 4 | 1 |
| 1:A:64:ASN:C | 1:A:66:GLU:N | 0.42 | 2.75 | 15 | 1 |
| 1:A:154:VAL:O | 1:A:158:PHE:N | 0.42 | 2.50 | 15 | 1 |
| 1:A:10:ILE:HG23 | 1:A:11:ALA:N | 0.42 | 2.29 | 17 | 1 |
| 1:A:15:ASP:OD1 | 1:A:19:GLU:OE2 | 0.42 | 2.36 | 5 | 1 |
| 1:A:99:ALA:O | 1:A:112:ASP:OD1 | 0.42 | 2.37 | 19 | 2 |
| 1:A:34:GLY:CA | 1:A:136:VAL:O | 0.42 | 2.68 | 3 | 12 |
| 1:A:21:ARG:NH2 | 1:A:23:ILE:HG22 | 0.42 | 2.29 | 15 | 4 |
| 1:A:150:THR:C | 1:A:152:ASP:N | 0.42 | 2.74 | 18 | 6 |
| 1:A:74:ASP:OD1 | 1:A:74:ASP:C | 0.42 | 2.62 | 10 | 1 |
| 1:A:46:LEU:CD2 | 1:A:46:LEU:C | 0.42 | 2.92 | 2 | 4 |
| 1:A:73:ASP:O | 1:A:74:ASP:OD1 | 0.42 | 2.38 | 10 | 1 |
| 1:A:153:GLU:OE1 | 1:A:154:VAL:N | 0.42 | 2.53 | 20 | 1 |
| 1:A:23:ILE:HD12 | 1:A:24:ALA:O | 0.42 | 2.15 | 1 | 4 |
| 1:A:97:PHE:CD1 | 1:A:97:PHE:N | 0.42 | 2.88 | 2 | 1 |
| 1:A:120:ASP:OD1 | 1:A:120:ASP:C | 0.42 | 2.63 | 5 | 1 |
| 1:A:44:MET:O | 1:A:48:GLU:CG | 0.42 | 2.67 | 18 | 1 |
| 1:A:36:ASP:O | 1:A:39:SER:OG | 0.42 | 2.38 | 15 | 1 |
| 1:A:129:GLN:CG | 1:A:130:ALA:N | 0.42 | 2.83 | 11 | 11 |
| 1:A:4:ASN:OD1 | 1:A:4:ASN:C | 0.42 | 2.63 | 20 | 1 |

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| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|------------------|------------------|----------|-------------|--------|-------|
| | | | | Worst | Total |
| 1:A:153:GLU:C | 1:A:153:GLU:OE1 | 0.41 | 2.63 | 1 | 3 |
| 1:A:105:ARG:HH22 | 1:A:111:PHE:C | 0.41 | 2.23 | 12 | 1 |
| 1:A:120:ASP:C | 1:A:120:ASP:OD1 | 0.41 | 2.62 | 17 | 1 |
| 1:A:100:PRO:O | 1:A:101:ALA:C | 0.41 | 2.63 | 9 | 1 |
| 1:A:120:ASP:O | 1:A:120:ASP:CG | 0.41 | 2.63 | 16 | 3 |
| 1:A:61:ILE:O | 1:A:61:ILE:CG2 | 0.41 | 2.68 | 16 | 1 |
| 1:A:74:ASP:OD1 | 1:A:74:ASP:N | 0.41 | 2.53 | 16 | 1 |
| 1:A:55:ASP:OD1 | 1:A:55:ASP:O | 0.41 | 2.38 | 5 | 2 |
| 1:A:160:ALA:O | 1:A:161:ALA:HB3 | 0.41 | 2.16 | 8 | 1 |
| 1:A:72:ILE:C | 1:A:74:ASP:N | 0.41 | 2.77 | 9 | 1 |
| 1:A:22:VAL:HG21 | 1:A:45:ARG:NH2 | 0.41 | 2.30 | 10 | 1 |
| 1:A:153:GLU:O | 1:A:154:VAL:C | 0.41 | 2.64 | 16 | 4 |
| 1:A:153:GLU:OE2 | 1:A:157:GLN:NE2 | 0.41 | 2.54 | 5 | 1 |
| 1:A:46:LEU:C | 1:A:46:LEU:CD2 | 0.41 | 2.93 | 10 | 2 |
| 1:A:56:LYS:N | 1:A:56:LYS:CD | 0.41 | 2.83 | 18 | 1 |
| 1:A:36:ASP:OD2 | 1:A:131:TYR:OH | 0.41 | 2.38 | 20 | 1 |
| 1:A:141:ASN:C | 1:A:141:ASN:OD1 | 0.41 | 2.64 | 17 | 1 |
| 1:A:55:ASP:CG | 1:A:110:ARG:CB | 0.41 | 2.94 | 5 | 2 |
| 1:A:74:ASP:OD1 | 1:A:74:ASP:O | 0.41 | 2.39 | 12 | 1 |
| 1:A:95:PHE:CB | 1:A:181:ALA:HB2 | 0.41 | 2.46 | 13 | 1 |
| 1:A:107:LEU:N | 1:A:107:LEU:HD22 | 0.41 | 2.31 | 14 | 1 |
| 1:A:35:CYS:O | 1:A:135:LEU:CD1 | 0.41 | 2.69 | 19 | 1 |
| 1:A:94:THR:HG22 | 1:A:115:ALA:HB1 | 0.41 | 1.93 | 4 | 1 |
| 1:A:76:MET:O | 1:A:81:GLN:OE1 | 0.41 | 2.39 | 13 | 1 |
| 1:A:78:THR:O | 1:A:79:ASP:C | 0.40 | 2.64 | 17 | 3 |
| 1:A:71:TYR:CD2 | 1:A:71:TYR:O | 0.40 | 2.74 | 16 | 1 |
| 1:A:73:ASP:OD2 | 1:A:98:PRO:O | 0.40 | 2.38 | 19 | 1 |
| 1:A:38:ASP:OD1 | 1:A:38:ASP:C | 0.40 | 2.63 | 18 | 1 |
| 1:A:49:LEU:HD23 | 1:A:49:LEU:H | 0.40 | 1.76 | 10 | 1 |
| 1:A:40:GLU:O | 1:A:41:THR:C | 0.40 | 2.63 | 8 | 1 |
| 1:A:121:HIS:N | 1:A:122:PRO:HD3 | 0.40 | 2.32 | 9 | 1 |
| 1:A:153:GLU:OE1 | 1:A:153:GLU:C | 0.40 | 2.65 | 10 | 1 |
| 1:A:106:TRP:CD1 | 1:A:106:TRP:H | 0.40 | 2.34 | 17 | 1 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

was analysed and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|---------------|--------------|-------------|-------------|----|
| 1 | A | 171/189 (90%) | 132±2 (77±1%) | 23±2 (13±1%) | 16±2 (9±1%) | 1 | 11 |
| All | All | 3420/3780 (90%) | 2640 (77%) | 461 (13%) | 319 (9%) | 1 | 11 |

All 34 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 | 52 | ARG | 20 |
| 1 | A | 57 | GLY | 20 |
| 1 | A | 58 | LEU | 20 |
| 1 | A | 121 | HIS | 20 |
| 1 | A | 146 | PRO | 20 |
| 1 | A | 160 | ALA | 20 |
| 1 | A | 162 | PHE | 20 |
| 1 | A | 48 | GLU | 19 |
| 1 | A | 122 | PRO | 19 |
| 1 | A | 134 | PRO | 19 |
| 1 | A | 89 | TRP | 16 |
| 1 | A | 91 | GLY | 14 |
| 1 | A | 37 | PRO | 12 |
| 1 | A | 154 | VAL | 11 |
| 1 | A | 105 | ARG | 11 |
| 1 | A | 144 | GLY | 10 |
| 1 | A | 21 | ARG | 7 |
| 1 | A | 153 | GLU | 7 |
| 1 | A | 109 | GLY | 6 |
| 1 | A | 166 | PRO | 4 |
| 1 | A | 101 | ALA | 4 |
| 1 | A | 111 | PHE | 3 |
| 1 | A | 112 | ASP | 3 |
| 1 | A | 38 | ASP | 3 |
| 1 | A | 110 | ARG | 2 |
| 1 | A | 143 | SER | 1 |
| 1 | A | 148 | CYS | 1 |
| 1 | A | 29 | ALA | 1 |
| 1 | A | 140 | ALA | 1 |
| 1 | A | 141 | ASN | 1 |
| 1 | A | 169 | THR | 1 |
| 1 | A | 31 | PHE | 1 |
| 1 | A | 100 | PRO | 1 |
| 1 | A | 147 | PRO | 1 |

6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|-----------------|---------------|-------------|-------------|
| 1 | A | 142/157 (90%) | 130±2 (92±1%) | 12±2 (8±1%) | 12 59 |
| All | All | 2840/3140 (90%) | 2599 (92%) | 241 (8%) | 12 59 |

All 33 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 | 58 | LEU | 20 |
| 1 | A | 78 | THR | 20 |
| 1 | A | 136 | VAL | 20 |
| 1 | A | 142 | LEU | 20 |
| 1 | A | 150 | THR | 20 |
| 1 | A | 129 | GLN | 16 |
| 1 | A | 107 | LEU | 15 |
| 1 | A | 183 | THR | 15 |
| 1 | A | 151 | VAL | 10 |
| 1 | A | 157 | GLN | 9 |
| 1 | A | 41 | THR | 8 |
| 1 | A | 153 | GLU | 7 |
| 1 | A | 114 | LEU | 7 |
| 1 | A | 21 | ARG | 7 |
| 1 | A | 46 | LEU | 6 |
| 1 | A | 110 | ARG | 5 |
| 1 | A | 25 | TYR | 5 |
| 1 | A | 40 | GLU | 4 |
| 1 | A | 67 | GLN | 4 |
| 1 | A | 35 | CYS | 3 |
| 1 | A | 138 | THR | 3 |
| 1 | A | 137 | SER | 3 |
| 1 | A | 127 | LEU | 3 |
| 1 | A | 95 | PHE | 2 |
| 1 | A | 96 | VAL | 1 |
| 1 | A | 48 | GLU | 1 |
| 1 | A | 73 | ASP | 1 |
| 1 | A | 165 | VAL | 1 |
| 1 | A | 141 | ASN | 1 |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1 | A | 81 | GLN | 1 |
| 1 | A | 43 | VAL | 1 |
| 1 | A | 54 | VAL | 1 |
| 1 | A | 169 | THR | 1 |

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 77% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping i

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

| | |
|---|------|
| Total number of shifts | 1971 |
| Number of shifts mapped to atoms | 1971 |
| 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 i

The following table shows the suggested chemical shift referencing corrections.

| Nucleus | # values | Correction \pm precision, ppm | Suggested action |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 187 | 0.04 ± 0.13 | None needed (< 0.5 ppm) |
| $^{13}\text{C}_\beta$ | 174 | 0.08 ± 0.12 | None needed (< 0.5 ppm) |
| $^{13}\text{C}'$ | 187 | 1.54 ± 0.12 | Should be applied |
| ^{15}N | 168 | -0.69 ± 0.38 | None needed (imprecise) |

7.1.3 Completeness of resonance assignments i

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 1806 atoms were assigned a chemical shift out of a possible 2317. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ^1H | ^{13}C | ^{15}N |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone | 819/837 (98%) | 324/338 (96%) | 340/342 (99%) | 155/157 (99%) |
| Sidechain | 987/1342 (74%) | 668/880 (76%) | 319/412 (77%) | 0/50 (0%) |

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| | Total | ¹ H | ¹³ C | ¹⁵ N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 0/138 (0%) | 0/67 (0%) | 0/67 (0%) | 0/4 (0%) |
| Overall | 1806/2317 (78%) | 992/1285 (77%) | 659/821 (80%) | 155/211 (73%) |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1968 atoms were assigned a chemical shift out of a possible 2552. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

| | Total | ¹ H | ¹³ C | ¹⁵ N |
|-----------|-----------------|-----------------|-----------------|-----------------|
| Backbone | 899/926 (97%) | 357/375 (95%) | 374/378 (99%) | 168/173 (97%) |
| Sidechain | 1069/1478 (72%) | 721/966 (75%) | 348/452 (77%) | 0/60 (0%) |
| Aromatic | 0/148 (0%) | 0/72 (0%) | 0/72 (0%) | 0/4 (0%) |
| Overall | 1968/2552 (77%) | 1078/1413 (76%) | 722/902 (80%) | 168/237 (71%) |

7.1.4 Statistically unusual chemical shifts [i](#)

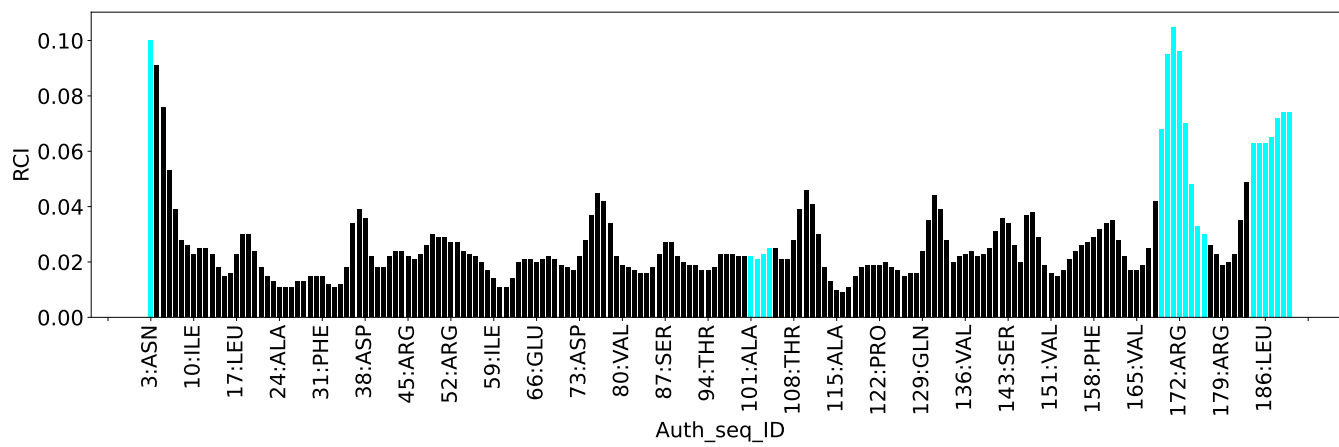
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1 | A | 104 | PRO | HG2 | -0.18 | 0.41 – 3.45 | -6.9 |
| 1 | A | 104 | PRO | HG3 | -0.03 | 0.33 – 3.48 | -6.2 |
| 1 | A | 85 | ILE | HD11 | -0.95 | -0.72 – 2.09 | -5.8 |
| 1 | A | 85 | ILE | HD12 | -0.95 | -0.72 – 2.09 | -5.8 |
| 1 | A | 85 | ILE | HD13 | -0.95 | -0.72 – 2.09 | -5.8 |
| 1 | A | 50 | LYS | CD | 23.14 | 23.50 – 34.42 | -5.3 |

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 | 1968 |
| Intra-residue ($ i-j =0$) | 390 |
| Sequential ($ i-j =1$) | 656 |
| Medium range ($ i-j >1$ and $ i-j <5$) | 444 |
| Long range ($ i-j \geq 5$) | 379 |
| Inter-chain | 0 |
| Hydrogen bond restraints | 99 |
| Disulfide bond restraints | 0 |
| Total dihedral-angle restraints | 187 |
| Number of unmapped restraints | 0 |
| Number of restraints per residue | 11.4 |
| Number of long range restraints per residue ¹ | 2.2 |

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) | 70.0 | 0.2 |
| 0.2-0.5 (Medium) | 52.6 | 0.5 |
| >0.5 (Large) | 0.1 | 0.56 |

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) | 14.2 | 5.58 |
| 10.0-20.0 (Medium) | None | None |
| >20.0 (Large) | None | None |

9 Distance violation analysis i

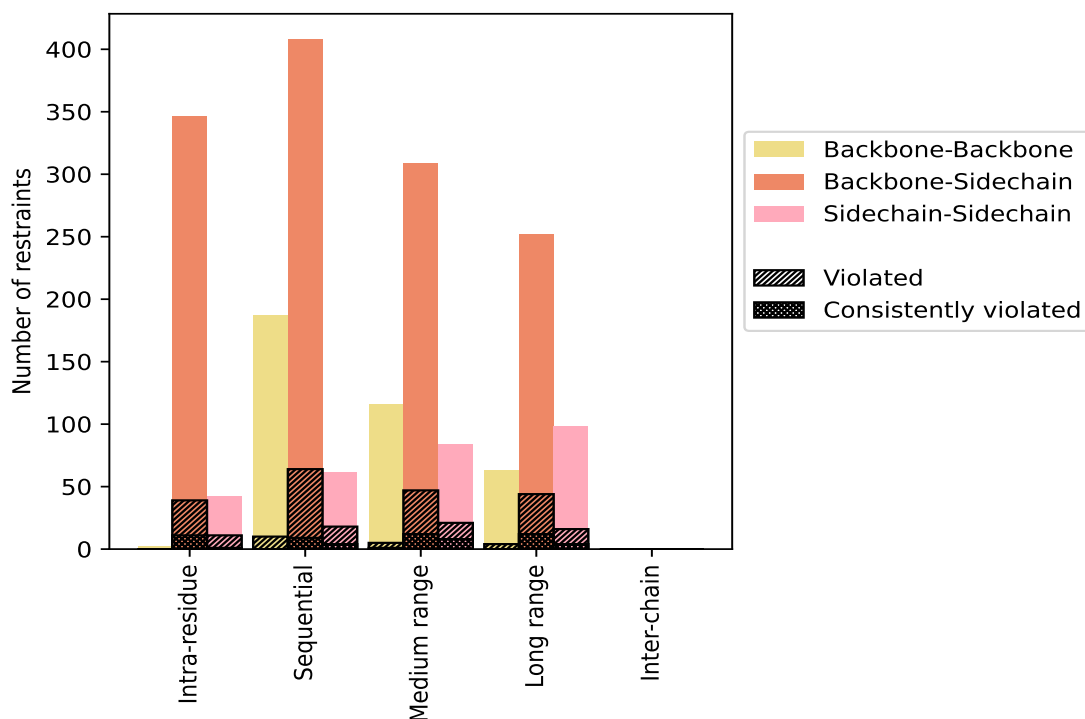
9.1 Summary of distance violations i

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

| Restrains type | Count | % ¹ | Violated ³ | | | Consistently Violated ⁴ | | |
|---|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
| | | | Count | % ² | % ¹ | Count | % ² | % ¹ |
| Intra-residue ($i-j =0$) | 390 | 19.8 | 50 | 12.8 | 2.5 | 12 | 3.1 | 0.6 |
| Backbone-Backbone | 2 | 0.1 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 346 | 17.6 | 39 | 11.3 | 2.0 | 11 | 3.2 | 0.6 |
| Sidechain-Sidechain | 42 | 2.1 | 11 | 26.2 | 0.6 | 1 | 2.4 | 0.1 |
| Sequential ($i-j =1$) | 656 | 33.3 | 92 | 14.0 | 4.7 | 13 | 2.0 | 0.7 |
| Backbone-Backbone | 187 | 9.5 | 10 | 5.3 | 0.5 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 408 | 20.7 | 64 | 15.7 | 3.3 | 9 | 2.2 | 0.5 |
| Sidechain-Sidechain | 61 | 3.1 | 18 | 29.5 | 0.9 | 4 | 6.6 | 0.2 |
| Medium range ($i-j >1$ & $i-j <5$) | 444 | 22.6 | 64 | 14.4 | 3.3 | 20 | 4.5 | 1.0 |
| Backbone-Backbone | 116 | 5.9 | 5 | 4.3 | 0.3 | 1 | 0.9 | 0.1 |
| Backbone-Sidechain | 244 | 12.4 | 38 | 15.6 | 1.9 | 11 | 4.5 | 0.6 |
| Sidechain-Sidechain | 84 | 4.3 | 21 | 25.0 | 1.1 | 8 | 9.5 | 0.4 |
| Long range ($i-j \geq 5$) | 379 | 19.3 | 58 | 15.3 | 2.9 | 14 | 3.7 | 0.7 |
| Backbone-Backbone | 63 | 3.2 | 4 | 6.3 | 0.2 | 0 | 0.0 | 0.0 |
| Backbone-Sidechain | 218 | 11.1 | 38 | 17.4 | 1.9 | 10 | 4.6 | 0.5 |
| Sidechain-Sidechain | 98 | 5.0 | 16 | 16.3 | 0.8 | 4 | 4.1 | 0.2 |
| 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 | 99 | 5.0 | 15 | 15.2 | 0.8 | 3 | 3.0 | 0.2 |
| Disulfide bond | 0 | 0.0 | 0 | 0.0 | 0.0 | 0 | 0.0 | 0.0 |
| Total | 1968 | 100.0 | 279 | 14.2 | 14.2 | 62 | 3.2 | 3.2 |
| Backbone-Backbone | 368 | 18.7 | 19 | 5.2 | 1.0 | 1 | 0.3 | 0.1 |
| Backbone-Sidechain | 1315 | 66.8 | 194 | 14.8 | 9.9 | 44 | 3.3 | 2.2 |
| Sidechain-Sidechain | 285 | 14.5 | 66 | 23.2 | 3.4 | 17 | 6.0 | 0.9 |

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

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



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

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

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

| Model ID | Number of violations | | | | | | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | | | | |
| 1 | 26 | 31 | 35 | 29 | 0 | 121 | 0.21 | 0.48 | 0.1 | 0.18 |
| 2 | 22 | 36 | 46 | 30 | 0 | 134 | 0.2 | 0.47 | 0.09 | 0.16 |
| 3 | 22 | 31 | 36 | 31 | 0 | 120 | 0.21 | 0.48 | 0.1 | 0.19 |
| 4 | 25 | 33 | 40 | 29 | 0 | 127 | 0.21 | 0.47 | 0.09 | 0.19 |
| 5 | 23 | 30 | 41 | 30 | 0 | 124 | 0.21 | 0.48 | 0.1 | 0.18 |
| 6 | 22 | 33 | 41 | 34 | 0 | 130 | 0.21 | 0.48 | 0.1 | 0.18 |
| 7 | 24 | 35 | 43 | 31 | 0 | 133 | 0.2 | 0.47 | 0.09 | 0.17 |
| 8 | 24 | 36 | 43 | 34 | 0 | 137 | 0.2 | 0.47 | 0.1 | 0.18 |
| 9 | 26 | 36 | 39 | 31 | 0 | 132 | 0.21 | 0.47 | 0.1 | 0.18 |
| 10 | 25 | 39 | 41 | 34 | 0 | 139 | 0.2 | 0.47 | 0.09 | 0.17 |

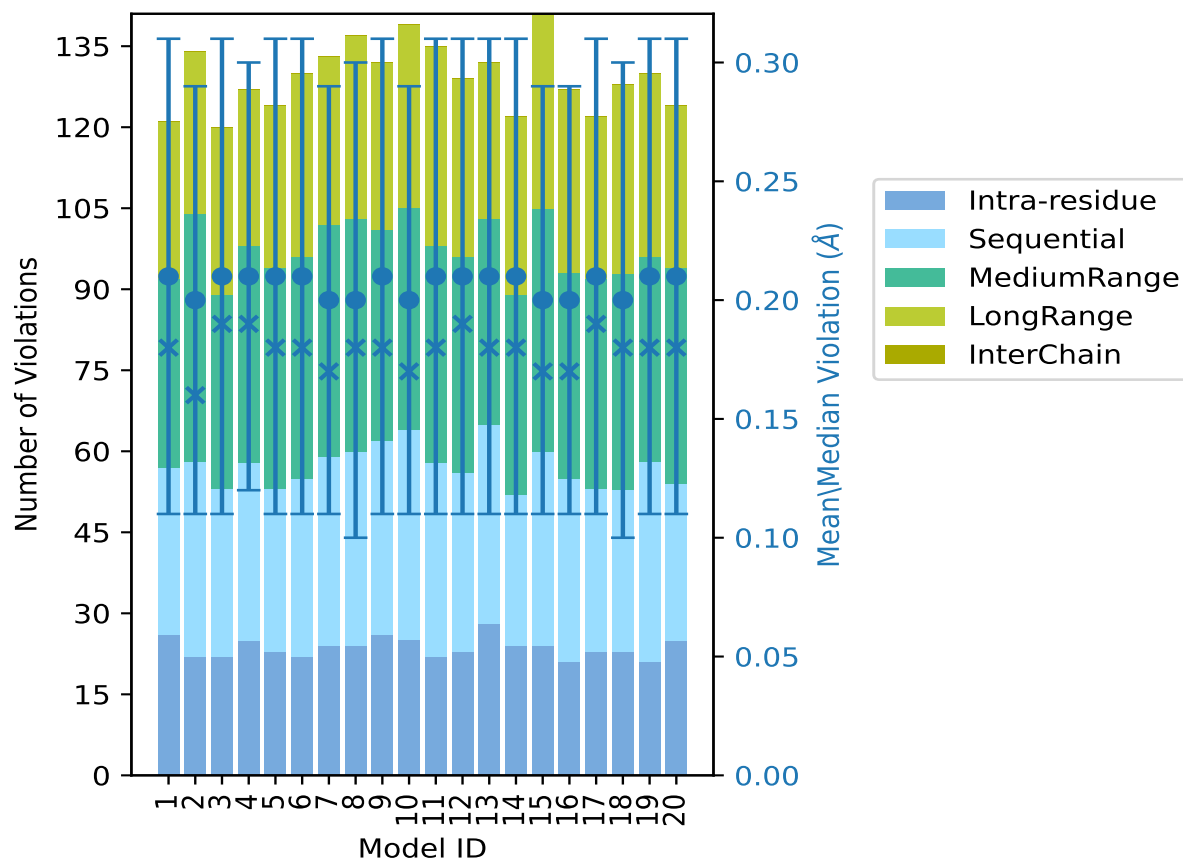
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| Model ID | Number of violations | | | | | Total | Mean (Å) | Max (Å) | SD ⁶ (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
| | IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | | | | | |
| 11 | 22 | 36 | 40 | 37 | 0 | 135 | 0.21 | 0.48 | 0.1 | 0.18 |
| 12 | 23 | 33 | 40 | 33 | 0 | 129 | 0.21 | 0.47 | 0.1 | 0.19 |
| 13 | 28 | 37 | 38 | 29 | 0 | 132 | 0.21 | 0.54 | 0.1 | 0.18 |
| 14 | 24 | 28 | 37 | 33 | 0 | 122 | 0.21 | 0.47 | 0.1 | 0.18 |
| 15 | 24 | 36 | 45 | 36 | 0 | 141 | 0.2 | 0.47 | 0.09 | 0.17 |
| 16 | 21 | 34 | 38 | 34 | 0 | 127 | 0.2 | 0.48 | 0.09 | 0.17 |
| 17 | 23 | 30 | 39 | 30 | 0 | 122 | 0.21 | 0.48 | 0.1 | 0.19 |
| 18 | 23 | 30 | 40 | 35 | 0 | 128 | 0.2 | 0.56 | 0.1 | 0.18 |
| 19 | 21 | 37 | 38 | 34 | 0 | 130 | 0.21 | 0.48 | 0.1 | 0.18 |
| 20 | 25 | 29 | 40 | 30 | 0 | 124 | 0.21 | 0.48 | 0.1 | 0.18 |

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints, ⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



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

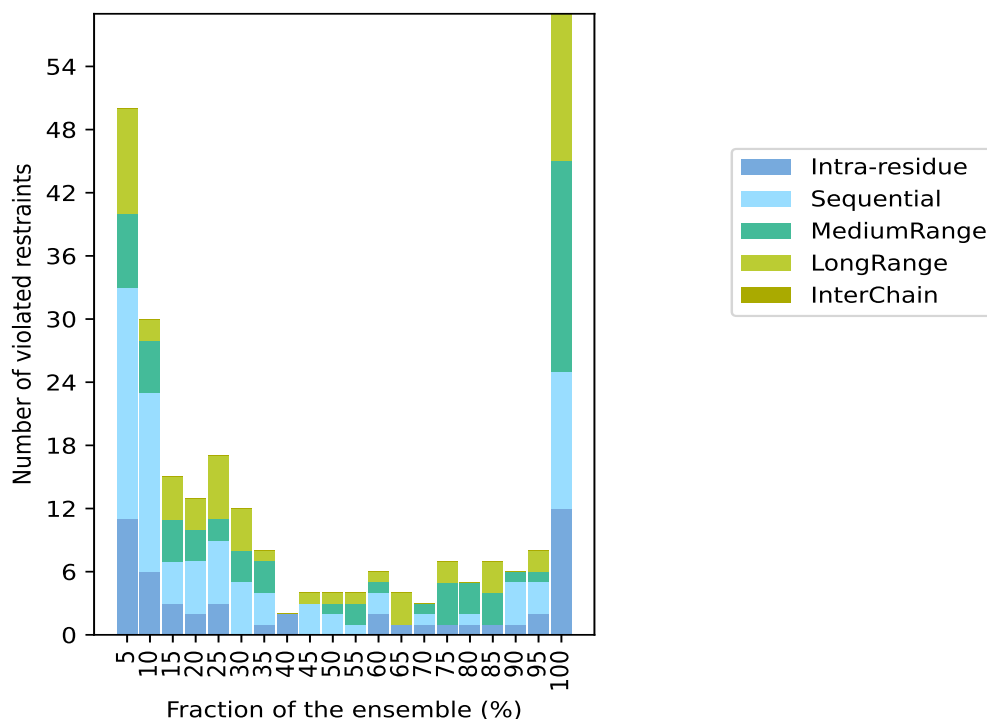
9.3 Distance violation statistics for the ensemble

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1605(IR:340, SQ:564, MR:380, LR:321, IC:0) restraints are not violated in the ensemble.

| Number of violated restraints | | | | | | Fraction of the ensemble | |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR ¹ | SQ ² | MR ³ | LR ⁴ | IC ⁵ | Total | Count ⁶ | % |
| 11 | 22 | 7 | 10 | 0 | 50 | 1 | 5.0 |
| 6 | 17 | 5 | 2 | 0 | 30 | 2 | 10.0 |
| 3 | 4 | 4 | 4 | 0 | 15 | 3 | 15.0 |
| 2 | 5 | 3 | 3 | 0 | 13 | 4 | 20.0 |
| 3 | 6 | 2 | 6 | 0 | 17 | 5 | 25.0 |
| 0 | 5 | 3 | 4 | 0 | 12 | 6 | 30.0 |
| 1 | 3 | 3 | 1 | 0 | 8 | 7 | 35.0 |
| 2 | 0 | 0 | 0 | 0 | 2 | 8 | 40.0 |
| 0 | 3 | 0 | 1 | 0 | 4 | 9 | 45.0 |
| 0 | 2 | 1 | 1 | 0 | 4 | 10 | 50.0 |
| 0 | 1 | 2 | 1 | 0 | 4 | 11 | 55.0 |
| 2 | 2 | 1 | 1 | 0 | 6 | 12 | 60.0 |
| 1 | 0 | 0 | 3 | 0 | 4 | 13 | 65.0 |
| 1 | 1 | 1 | 0 | 0 | 3 | 14 | 70.0 |
| 1 | 0 | 4 | 2 | 0 | 7 | 15 | 75.0 |
| 1 | 1 | 3 | 0 | 0 | 5 | 16 | 80.0 |
| 1 | 0 | 3 | 3 | 0 | 7 | 17 | 85.0 |
| 1 | 4 | 1 | 0 | 0 | 6 | 18 | 90.0 |
| 2 | 3 | 1 | 2 | 0 | 8 | 19 | 95.0 |
| 12 | 13 | 20 | 14 | 0 | 59 | 20 | 100.0 |

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

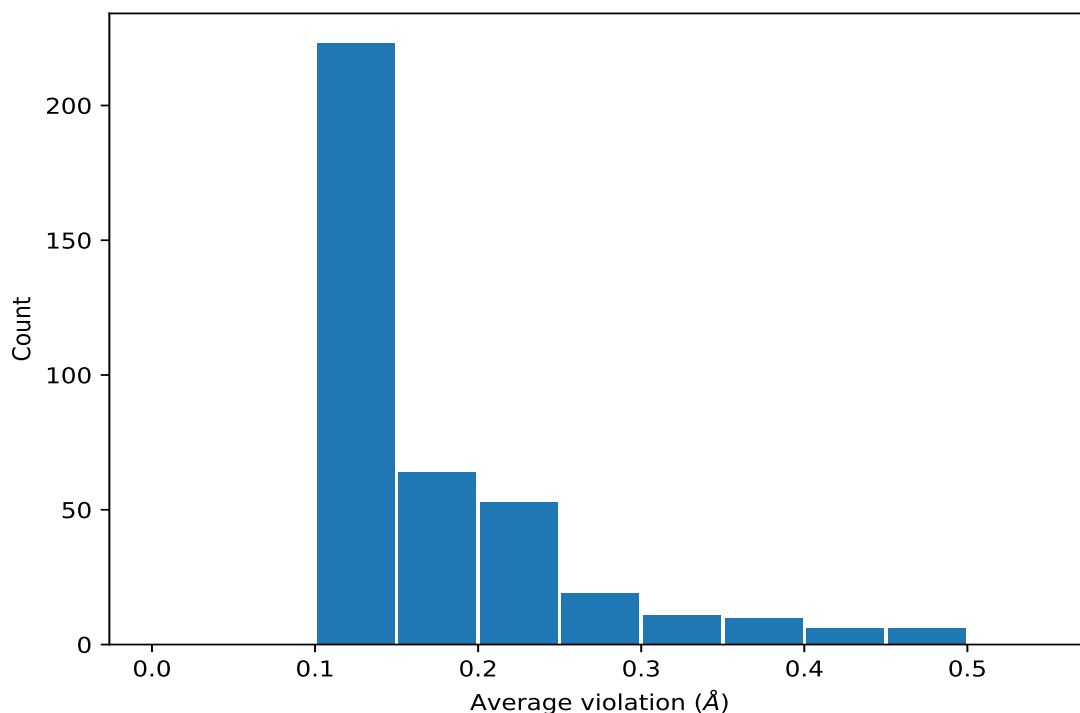
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 20 | 0.47 | 0.0 | 0.47 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 20 | 0.41 | 0.01 | 0.41 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 20 | 0.41 | 0.03 | 0.4 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 20 | 0.4 | 0.02 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 20 | 0.4 | 0.01 | 0.4 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 20 | 0.4 | 0.04 | 0.42 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 20 | 0.38 | 0.01 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 20 | 0.38 | 0.04 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 20 | 0.38 | 0.04 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 20 | 0.38 | 0.04 | 0.38 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 20 | 0.38 | 0.04 | 0.35 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 20 | 0.38 | 0.01 | 0.38 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 20 | 0.37 | 0.02 | 0.37 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 20 | 0.37 | 0.03 | 0.37 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 20 | 0.36 | 0.06 | 0.39 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 20 | 0.33 | 0.02 | 0.33 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 20 | 0.32 | 0.04 | 0.32 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 20 | 0.32 | 0.02 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 20 | 0.32 | 0.05 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 20 | 0.32 | 0.05 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 20 | 0.32 | 0.05 | 0.33 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 20 | 0.32 | 0.02 | 0.31 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 20 | 0.32 | 0.03 | 0.32 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 20 | 0.29 | 0.05 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 20 | 0.29 | 0.05 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 20 | 0.29 | 0.05 | 0.27 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 20 | 0.29 | 0.01 | 0.29 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 20 | 0.28 | 0.04 | 0.29 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 20 | 0.26 | 0.03 | 0.28 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 20 | 0.24 | 0.01 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 20 | 0.24 | 0.02 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 20 | 0.24 | 0.02 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 20 | 0.24 | 0.02 | 0.25 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 20 | 0.24 | 0.03 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 20 | 0.23 | 0.01 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 20 | 0.23 | 0.01 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 20 | 0.23 | 0.01 | 0.23 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 20 | 0.23 | 0.01 | 0.23 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 20 | 0.23 | 0.02 | 0.24 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 20 | 0.23 | 0.03 | 0.24 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 20 | 0.23 | 0.01 | 0.23 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 20 | 0.23 | 0.03 | 0.23 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 20 | 0.22 | 0.01 | 0.22 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 20 | 0.22 | 0.03 | 0.22 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 20 | 0.22 | 0.05 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 20 | 0.22 | 0.01 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 20 | 0.22 | 0.01 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 20 | 0.22 | 0.01 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 20 | 0.22 | 0.01 | 0.22 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 20 | 0.21 | 0.02 | 0.22 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 20 | 0.21 | 0.02 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 20 | 0.21 | 0.02 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 20 | 0.21 | 0.02 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 20 | 0.21 | 0.02 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 20 | 0.21 | 0.01 | 0.21 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 20 | 0.21 | 0.03 | 0.21 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 20 | 0.21 | 0.02 | 0.2 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 20 | 0.2 | 0.03 | 0.2 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 20 | 0.2 | 0.02 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 20 | 0.2 | 0.02 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 20 | 0.2 | 0.02 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 20 | 0.2 | 0.02 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 20 | 0.2 | 0.02 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 20 | 0.2 | 0.02 | 0.2 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 20 | 0.2 | 0.02 | 0.2 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 20 | 0.19 | 0.02 | 0.2 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 20 | 0.18 | 0.03 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 20 | 0.18 | 0.03 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 20 | 0.18 | 0.03 | 0.19 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 20 | 0.17 | 0.03 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 20 | 0.17 | 0.03 | 0.16 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 20 | 0.17 | 0.03 | 0.16 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 20 | 0.17 | 0.03 | 0.16 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 20 | 0.17 | 0.03 | 0.16 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 20 | 0.17 | 0.02 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 20 | 0.16 | 0.02 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 20 | 0.16 | 0.02 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 20 | 0.16 | 0.02 | 0.16 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 20 | 0.16 | 0.01 | 0.16 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 20 | 0.16 | 0.01 | 0.16 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 20 | 0.16 | 0.01 | 0.16 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 20 | 0.16 | 0.02 | 0.16 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 20 | 0.16 | 0.01 | 0.15 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 20 | 0.16 | 0.02 | 0.16 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 20 | 0.16 | 0.02 | 0.16 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 20 | 0.13 | 0.0 | 0.13 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 20 | 0.13 | 0.02 | 0.13 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 20 | 0.13 | 0.02 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 20 | 0.13 | 0.02 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 20 | 0.13 | 0.02 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 20 | 0.13 | 0.02 | 0.12 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 19 | 0.47 | 0.01 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 19 | 0.47 | 0.01 | 0.47 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 19 | 0.47 | 0.01 | 0.47 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 19 | 0.21 | 0.03 | 0.21 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 19 | 0.21 | 0.02 | 0.21 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 19 | 0.18 | 0.03 | 0.18 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 19 | 0.18 | 0.03 | 0.18 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 19 | 0.18 | 0.03 | 0.18 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 19 | 0.18 | 0.01 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 19 | 0.17 | 0.03 | 0.17 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 19 | 0.17 | 0.03 | 0.17 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 19 | 0.17 | 0.03 | 0.17 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 19 | 0.15 | 0.03 | 0.15 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 19 | 0.12 | 0.0 | 0.12 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 18 | 0.3 | 0.02 | 0.3 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 18 | 0.26 | 0.06 | 0.26 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 18 | 0.19 | 0.02 | 0.19 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 18 | 0.14 | 0.02 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 18 | 0.14 | 0.02 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 18 | 0.14 | 0.02 | 0.14 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 18 | 0.13 | 0.01 | 0.13 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 18 | 0.12 | 0.02 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 18 | 0.12 | 0.01 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 18 | 0.12 | 0.01 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 18 | 0.12 | 0.01 | 0.12 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 17 | 0.15 | 0.02 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 17 | 0.15 | 0.01 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 17 | 0.15 | 0.01 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 17 | 0.15 | 0.01 | 0.15 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 17 | 0.14 | 0.02 | 0.14 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 17 | 0.14 | 0.03 | 0.13 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 17 | 0.13 | 0.01 | 0.13 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 17 | 0.12 | 0.02 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 17 | 0.12 | 0.02 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 17 | 0.12 | 0.02 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 17 | 0.12 | 0.01 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 17 | 0.12 | 0.01 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 17 | 0.12 | 0.01 | 0.11 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 16 | 0.2 | 0.06 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 16 | 0.17 | 0.04 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 16 | 0.17 | 0.04 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 16 | 0.17 | 0.04 | 0.18 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 16 | 0.14 | 0.02 | 0.14 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 16 | 0.14 | 0.02 | 0.14 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 16 | 0.14 | 0.02 | 0.14 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 16 | 0.14 | 0.03 | 0.13 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 16 | 0.13 | 0.02 | 0.13 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 15 | 0.15 | 0.03 | 0.14 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 15 | 0.15 | 0.02 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 15 | 0.15 | 0.02 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 15 | 0.15 | 0.02 | 0.15 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 15 | 0.14 | 0.02 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 15 | 0.13 | 0.01 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 15 | 0.13 | 0.01 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 15 | 0.13 | 0.01 | 0.13 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 15 | 0.12 | 0.02 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 15 | 0.12 | 0.01 | 0.12 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 15 | 0.11 | 0.01 | 0.11 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 14 | 0.46 | 0.0 | 0.46 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 14 | 0.18 | 0.02 | 0.19 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 14 | 0.17 | 0.05 | 0.17 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 13 | 0.33 | 0.1 | 0.34 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 13 | 0.13 | 0.02 | 0.12 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 13 | 0.12 | 0.02 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 13 | 0.12 | 0.02 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 13 | 0.12 | 0.02 | 0.13 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 13 | 0.11 | 0.01 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 13 | 0.11 | 0.01 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 13 | 0.11 | 0.01 | 0.11 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 12 | 0.39 | 0.02 | 0.4 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 12 | 0.25 | 0.01 | 0.25 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 12 | 0.14 | 0.04 | 0.12 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 12 | 0.13 | 0.02 | 0.12 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 12 | 0.12 | 0.01 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 12 | 0.12 | 0.01 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 12 | 0.12 | 0.01 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 12 | 0.12 | 0.01 | 0.12 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 12 | 0.11 | 0.01 | 0.11 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 11 | 0.13 | 0.03 | 0.13 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 11 | 0.13 | 0.02 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 11 | 0.13 | 0.02 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 11 | 0.13 | 0.02 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 11 | 0.12 | 0.01 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 11 | 0.12 | 0.01 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 11 | 0.12 | 0.01 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 11 | 0.11 | 0.01 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 11 | 0.11 | 0.01 | 0.11 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 11 | 0.11 | 0.01 | 0.11 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 10 | 0.13 | 0.02 | 0.14 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 10 | 0.12 | 0.02 | 0.12 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 10 | 0.12 | 0.02 | 0.12 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 10 | 0.12 | 0.02 | 0.12 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 10 | 0.12 | 0.01 | 0.12 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 10 | 0.11 | 0.01 | 0.11 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 9 | 0.43 | 0.01 | 0.43 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 9 | 0.24 | 0.17 | 0.15 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 9 | 0.24 | 0.17 | 0.15 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 9 | 0.24 | 0.17 | 0.15 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 9 | 0.14 | 0.02 | 0.14 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 9 | 0.14 | 0.02 | 0.13 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 9 | 0.14 | 0.02 | 0.13 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 9 | 0.14 | 0.02 | 0.13 |
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 8 | 0.12 | 0.01 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 8 | 0.12 | 0.01 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 8 | 0.12 | 0.01 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 8 | 0.12 | 0.01 | 0.12 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 7 | 0.3 | 0.0 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 7 | 0.3 | 0.0 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 7 | 0.3 | 0.0 | 0.3 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 7 | 0.24 | 0.05 | 0.25 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 7 | 0.24 | 0.05 | 0.25 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 7 | 0.24 | 0.05 | 0.25 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 7 | 0.17 | 0.02 | 0.17 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 7 | 0.14 | 0.02 | 0.14 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 7 | 0.12 | 0.01 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 7 | 0.12 | 0.01 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 7 | 0.12 | 0.01 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 7 | 0.12 | 0.01 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 7 | 0.12 | 0.01 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 7 | 0.12 | 0.01 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 7 | 0.12 | 0.01 | 0.12 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 7 | 0.12 | 0.01 | 0.12 |
| (2,238) | 1:170:A:GLY:HA3 | 1:171:A:GLY:H | 6 | 0.23 | 0.04 | 0.24 |
| (2,1588) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG2 | 6 | 0.16 | 0.03 | 0.16 |
| (2,1617) | 1:47:A:LEU:HA | 1:54:A:VAL:HB | 6 | 0.16 | 0.06 | 0.13 |
| (2,1281) | 1:16:A:VAL:H | 1:21:A:ARG:HD2 | 6 | 0.14 | 0.06 | 0.12 |
| (2,1681) | 1:108:A:THR:HG21 | 1:109:A:GLY:HA2 | 6 | 0.14 | 0.03 | 0.13 |
| (2,1681) | 1:108:A:THR:HG22 | 1:109:A:GLY:HA2 | 6 | 0.14 | 0.03 | 0.13 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1681) | 1:108:A:THR:HG23 | 1:109:A:GLY:HA2 | 6 | 0.14 | 0.03 | 0.13 |
| (2,720) | 1:104:A:PRO:HG2 | 1:105:A:ARG:H | 6 | 0.14 | 0.02 | 0.14 |
| (1,36) | 1:65:A:TYR:O | 1:69:A:LYS:H | 6 | 0.13 | 0.03 | 0.13 |
| (2,766) | 1:46:A:LEU:HG | 1:47:A:LEU:H | 6 | 0.13 | 0.02 | 0.14 |
| (2,930) | 1:62:A:ALA:HB1 | 1:68:A:LEU:H | 6 | 0.12 | 0.02 | 0.12 |
| (2,930) | 1:62:A:ALA:HB2 | 1:68:A:LEU:H | 6 | 0.12 | 0.02 | 0.12 |
| (2,930) | 1:62:A:ALA:HB3 | 1:68:A:LEU:H | 6 | 0.12 | 0.02 | 0.12 |
| (2,660) | 1:105:A:ARG:H | 1:107:A:LEU:HG | 6 | 0.12 | 0.02 | 0.12 |
| (1,20) | 1:13:A:ALA:O | 1:17:A:LEU:H | 6 | 0.11 | 0.01 | 0.12 |
| (2,672) | 1:46:A:LEU:HA | 1:49:A:LEU:H | 6 | 0.11 | 0.01 | 0.11 |
| (2,1471) | 1:27:A:THR:HA | 1:28:A:GLU:HG2 | 6 | 0.11 | 0.01 | 0.12 |
| (2,1683) | 1:118:A:VAL:HG11 | 1:120:A:ASP:HB3 | 6 | 0.1 | 0.01 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG12 | 1:120:A:ASP:HB3 | 6 | 0.1 | 0.01 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG13 | 1:120:A:ASP:HB3 | 6 | 0.1 | 0.01 | 0.1 |
| (2,833) | 1:106:A:TRP:H | 1:106:A:TRP:HB3 | 5 | 0.35 | 0.01 | 0.35 |
| (2,1299) | 1:19:A:GLU:HB3 | 1:19:A:GLU:HG3 | 5 | 0.31 | 0.0 | 0.31 |
| (2,1151) | 1:107:A:LEU:HD21 | 1:108:A:THR:HA | 5 | 0.25 | 0.01 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD22 | 1:108:A:THR:HA | 5 | 0.25 | 0.01 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD23 | 1:108:A:THR:HA | 5 | 0.25 | 0.01 | 0.25 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD11 | 5 | 0.23 | 0.03 | 0.25 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD12 | 5 | 0.23 | 0.03 | 0.25 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD13 | 5 | 0.23 | 0.03 | 0.25 |
| (2,51) | 1:179:A:ARG:HG2 | 1:180:A:ASP:H | 5 | 0.22 | 0.06 | 0.2 |
| (2,1275) | 1:16:A:VAL:HG11 | 1:21:A:ARG:HD2 | 5 | 0.18 | 0.01 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG12 | 1:21:A:ARG:HD2 | 5 | 0.18 | 0.01 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG13 | 1:21:A:ARG:HD2 | 5 | 0.18 | 0.01 | 0.18 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD21 | 5 | 0.15 | 0.01 | 0.15 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD22 | 5 | 0.15 | 0.01 | 0.15 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD23 | 5 | 0.15 | 0.01 | 0.15 |
| (1,30) | 1:42:A:ALA:O | 1:46:A:LEU:H | 5 | 0.14 | 0.01 | 0.14 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD21 | 5 | 0.13 | 0.0 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD22 | 5 | 0.13 | 0.0 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD23 | 5 | 0.13 | 0.0 | 0.13 |
| (2,433) | 1:37:A:PRO:HG2 | 1:38:A:ASP:H | 5 | 0.13 | 0.02 | 0.12 |
| (2,1519) | 1:19:A:GLU:HA | 1:21:A:ARG:HD3 | 5 | 0.12 | 0.02 | 0.12 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD21 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD22 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD23 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD21 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD22 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD23 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD21 | 5 | 0.12 | 0.02 | 0.11 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD22 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD23 | 5 | 0.12 | 0.02 | 0.11 |
| (2,1715) | 1:154:A:VAL:HG11 | 1:164:A:VAL:HA | 5 | 0.12 | 0.01 | 0.12 |
| (2,1715) | 1:154:A:VAL:HG12 | 1:164:A:VAL:HA | 5 | 0.12 | 0.01 | 0.12 |
| (2,1715) | 1:154:A:VAL:HG13 | 1:164:A:VAL:HA | 5 | 0.12 | 0.01 | 0.12 |
| (2,980) | 1:55:A:ASP:HB3 | 1:56:A:LYS:HA | 5 | 0.12 | 0.01 | 0.12 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG21 | 5 | 0.12 | 0.01 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG22 | 5 | 0.12 | 0.01 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG23 | 5 | 0.12 | 0.01 | 0.11 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG11 | 5 | 0.12 | 0.01 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG12 | 5 | 0.12 | 0.01 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG13 | 5 | 0.12 | 0.01 | 0.12 |
| (2,1009) | 1:55:A:ASP:HB2 | 1:110:A:ARG:HA | 5 | 0.11 | 0.01 | 0.12 |
| (2,1012) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HA | 5 | 0.11 | 0.0 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HA | 5 | 0.11 | 0.0 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HA | 5 | 0.11 | 0.0 | 0.11 |
| (2,1242) | 1:188:A:ARG:HG2 | 1:189:A:GLN:HA | 4 | 0.21 | 0.01 | 0.2 |
| (2,1826) | 1:188:A:ARG:HG2 | 1:188:A:ARG:HD3 | 4 | 0.2 | 0.0 | 0.2 |
| (2,1587) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG3 | 4 | 0.16 | 0.04 | 0.16 |
| (2,1615) | 1:148:A:CYS:H | 1:149:A:ARG:HB3 | 4 | 0.16 | 0.02 | 0.16 |
| (2,412) | 1:75:A:THR:H | 1:76:A:MET:HG3 | 4 | 0.13 | 0.01 | 0.13 |
| (2,909) | 1:42:A:ALA:HB1 | 1:45:A:ARG:HD3 | 4 | 0.12 | 0.01 | 0.12 |
| (2,909) | 1:42:A:ALA:HB2 | 1:45:A:ARG:HD3 | 4 | 0.12 | 0.01 | 0.12 |
| (2,909) | 1:42:A:ALA:HB3 | 1:45:A:ARG:HD3 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG21 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG22 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG23 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG21 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG22 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG23 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG21 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG22 | 4 | 0.12 | 0.01 | 0.12 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG23 | 4 | 0.12 | 0.01 | 0.12 |
| (2,836) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 4 | 0.12 | 0.01 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD11 | 4 | 0.12 | 0.0 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD12 | 4 | 0.12 | 0.0 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD13 | 4 | 0.12 | 0.0 | 0.12 |
| (2,39) | 1:103:A:THR:H | 1:104:A:PRO:HD2 | 4 | 0.11 | 0.0 | 0.11 |
| (2,1446) | 1:62:A:ALA:HA | 1:128:A:CYS:HB2 | 4 | 0.11 | 0.01 | 0.12 |
| (2,101) | 1:151:A:VAL:H | 1:154:A:VAL:H | 4 | 0.11 | 0.01 | 0.11 |
| (2,333) | 1:27:A:THR:H | 1:30:A:VAL:H | 4 | 0.11 | 0.01 | 0.11 |
| (2,29) | 1:179:A:ARG:H | 1:179:A:ARG:HD2 | 3 | 0.3 | 0.01 | 0.3 |

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| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1288) | 1:105:A:ARG:HB2 | 1:105:A:ARG:HD3 | 3 | 0.19 | 0.0 | 0.19 |
| (2,366) | 1:171:A:GLY:H | 1:172:A:ARG:HB3 | 3 | 0.15 | 0.03 | 0.13 |
| (2,1110) | 1:84:A:THR:HA | 1:88:A:ARG:HB3 | 3 | 0.15 | 0.05 | 0.13 |
| (2,148) | 1:51:A:GLN:H | 1:51:A:GLN:HB3 | 3 | 0.12 | 0.01 | 0.11 |
| (2,845) | 1:105:A:ARG:HB2 | 1:109:A:GLY:H | 3 | 0.12 | 0.01 | 0.12 |
| (2,1755) | 1:186:A:LEU:HD21 | 1:187:A:PHE:HA | 3 | 0.12 | 0.01 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD22 | 1:187:A:PHE:HA | 3 | 0.12 | 0.01 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD23 | 1:187:A:PHE:HA | 3 | 0.12 | 0.01 | 0.13 |
| (1,37) | 1:67:A:GLN:O | 1:71:A:TYR:N | 3 | 0.12 | 0.0 | 0.12 |
| (1,90) | 1:97:A:PHE:N | 1:114:A:LEU:O | 3 | 0.12 | 0.01 | 0.11 |
| (2,530) | 1:73:A:ASP:HB2 | 1:74:A:ASP:H | 3 | 0.12 | 0.01 | 0.12 |
| (2,61) | 1:60:A:LEU:HA | 1:117:A:ARG:H | 3 | 0.11 | 0.01 | 0.12 |
| (2,1422) | 1:48:A:GLU:HB3 | 1:50:A:LYS:H | 3 | 0.11 | 0.01 | 0.1 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG21 | 3 | 0.11 | 0.0 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG22 | 3 | 0.11 | 0.0 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG23 | 3 | 0.11 | 0.0 | 0.11 |
| (2,1771) | 1:17:A:LEU:HD11 | 1:18:A:ASN:HA | 3 | 0.11 | 0.01 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD12 | 1:18:A:ASN:HA | 3 | 0.11 | 0.01 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD13 | 1:18:A:ASN:HA | 3 | 0.11 | 0.01 | 0.1 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD11 | 3 | 0.11 | 0.01 | 0.11 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD12 | 3 | 0.11 | 0.01 | 0.11 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD13 | 3 | 0.11 | 0.01 | 0.11 |
| (1,84) | 1:61:A:ILE:H | 1:135:A:LEU:O | 3 | 0.1 | 0.0 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG21 | 1:134:A:PRO:HB3 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG22 | 1:134:A:PRO:HB3 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG23 | 1:134:A:PRO:HB3 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG11 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG12 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG13 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG11 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG12 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG13 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG11 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG12 | 3 | 0.1 | 0.0 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG13 | 3 | 0.1 | 0.0 | 0.1 |
| (2,82) | 1:77:A:LEU:H | 1:77:A:LEU:HB3 | 2 | 0.45 | 0.01 | 0.45 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG21 | 2 | 0.28 | 0.0 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG22 | 2 | 0.28 | 0.0 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG23 | 2 | 0.28 | 0.0 | 0.28 |
| (2,1523) | 1:172:A:ARG:H | 1:173:A:LEU:HA | 2 | 0.2 | 0.0 | 0.2 |
| (2,402) | 1:184:A:GLY:H | 1:185:A:GLU:HB3 | 2 | 0.19 | 0.0 | 0.19 |
| (2,723) | 1:76:A:MET:HG3 | 1:77:A:LEU:H | 2 | 0.19 | 0.04 | 0.19 |

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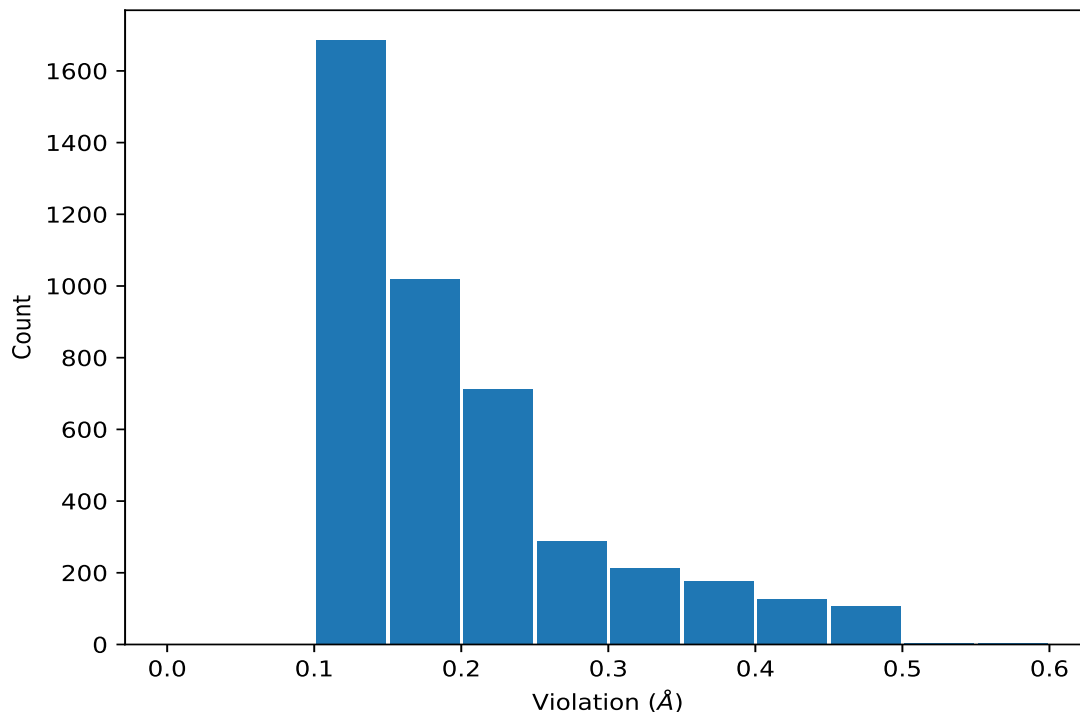
| Key | Atom-1 | Atom-2 | Models ¹ | Mean (Å) | SD ¹ (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD21 | 2 | 0.19 | 0.0 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD22 | 2 | 0.19 | 0.0 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD23 | 2 | 0.19 | 0.0 | 0.19 |
| (2,1023) | 1:179:A:ARG:HB2 | 1:181:A:ALA:HA | 2 | 0.18 | 0.0 | 0.18 |
| (2,1144) | 1:183:A:THR:HG21 | 1:185:A:GLU:HB3 | 2 | 0.17 | 0.01 | 0.17 |
| (2,1144) | 1:183:A:THR:HG22 | 1:185:A:GLU:HB3 | 2 | 0.17 | 0.01 | 0.17 |
| (2,1144) | 1:183:A:THR:HG23 | 1:185:A:GLU:HB3 | 2 | 0.17 | 0.01 | 0.17 |
| (2,1109) | 1:177:A:GLU:HB3 | 1:178:A:ILE:HA | 2 | 0.16 | 0.02 | 0.16 |
| (2,1478) | 1:30:A:VAL:HG11 | 1:31:A:PHE:HA | 2 | 0.16 | 0.01 | 0.16 |
| (2,1478) | 1:30:A:VAL:HG12 | 1:31:A:PHE:HA | 2 | 0.16 | 0.01 | 0.16 |
| (2,1478) | 1:30:A:VAL:HG13 | 1:31:A:PHE:HA | 2 | 0.16 | 0.01 | 0.16 |
| (1,34) | 1:44:A:MET:O | 1:48:A:GLU:H | 2 | 0.16 | 0.02 | 0.16 |
| (2,87) | 1:81:A:GLN:H | 1:81:A:GLN:HB3 | 2 | 0.16 | 0.01 | 0.16 |
| (2,365) | 1:171:A:GLY:H | 1:172:A:ARG:HD2 | 2 | 0.15 | 0.02 | 0.15 |
| (2,1073) | 1:115:A:ALA:H | 1:116:A:VAL:HB | 2 | 0.15 | 0.02 | 0.15 |
| (2,1316) | 1:6:A:GLN:HG2 | 1:7:A:ARG:H | 2 | 0.15 | 0.02 | 0.15 |
| (2,928) | 1:62:A:ALA:HB1 | 1:68:A:LEU:HA | 2 | 0.14 | 0.01 | 0.14 |
| (2,928) | 1:62:A:ALA:HB2 | 1:68:A:LEU:HA | 2 | 0.14 | 0.01 | 0.14 |
| (2,928) | 1:62:A:ALA:HB3 | 1:68:A:LEU:HA | 2 | 0.14 | 0.01 | 0.14 |
| (2,144) | 1:78:A:THR:HG21 | 1:82:A:ARG:H | 2 | 0.13 | 0.02 | 0.13 |
| (2,144) | 1:78:A:THR:HG22 | 1:82:A:ARG:H | 2 | 0.13 | 0.02 | 0.13 |
| (2,144) | 1:78:A:THR:HG23 | 1:82:A:ARG:H | 2 | 0.13 | 0.02 | 0.13 |
| (2,165) | 1:176:A:SER:H | 1:177:A:GLU:HG3 | 2 | 0.13 | 0.0 | 0.13 |
| (2,1589) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HB3 | 2 | 0.13 | 0.0 | 0.13 |
| (2,170) | 1:173:A:LEU:HB2 | 1:174:A:ASN:H | 2 | 0.12 | 0.02 | 0.12 |
| (2,209) | 1:90:A:PRO:HD3 | 1:91:A:GLY:H | 2 | 0.12 | 0.01 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD21 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD22 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD23 | 2 | 0.12 | 0.0 | 0.12 |
| (2,383) | 1:158:A:PHE:HB2 | 1:159:A:GLY:H | 2 | 0.12 | 0.02 | 0.12 |
| (2,1064) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1064) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1064) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HE2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1502) | 1:79:A:ASP:HA | 1:82:A:ARG:HB2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,1858) | 1:63:A:ALA:H | 1:67:A:GLN:HG2 | 2 | 0.12 | 0.0 | 0.12 |
| (2,274) | 1:112:A:ASP:H | 1:112:A:ASP:HB3 | 2 | 0.11 | 0.0 | 0.11 |
| (2,611) | 1:163:A:PRO:HA | 1:164:A:VAL:H | 2 | 0.11 | 0.01 | 0.11 |
| (2,1302) | 1:185:A:GLU:HB3 | 1:185:A:GLU:HG2 | 2 | 0.11 | 0.0 | 0.11 |
| (2,1585) | 1:54:A:VAL:H | 1:55:A:ASP:HB3 | 2 | 0.11 | 0.01 | 0.11 |
| (2,15) | 1:96:A:VAL:HB | 1:97:A:PHE:H | 2 | 0.11 | 0.0 | 0.11 |

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 18 | 0.56 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 18 | 0.56 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 18 | 0.56 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 13 | 0.54 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 13 | 0.54 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 13 | 0.54 |
| (2,1827) | 1:188:A:ARG:HA | 1:188:A:ARG:HD3 | 13 | 0.5 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 3 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 3 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 3 | 0.48 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 5 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 5 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 5 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 11 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 11 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 11 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 19 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 19 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 19 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 20 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 20 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 20 | 0.48 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 3 | 0.48 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 6 | 0.48 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 16 | 0.48 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 17 | 0.48 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 1 | 0.48 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 1 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 1 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 1 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 4 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 4 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 4 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 6 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 6 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 6 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 7 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 7 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 7 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 8 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 8 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 8 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 9 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 9 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 9 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 10 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 10 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 10 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 12 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 12 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 12 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 13 | 0.47 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 13 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 13 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 14 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 14 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 14 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 15 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 15 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 15 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 17 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 17 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 17 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 18 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 18 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 18 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 1 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 2 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 4 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 5 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 7 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 8 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 9 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 10 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 11 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 12 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 13 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 14 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 15 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 17 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 18 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 19 | 0.47 |
| (2,1480) | 1:129:A:GLN:HA | 1:129:A:GLN:HG2 | 20 | 0.47 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 3 | 0.47 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD11 | 16 | 0.46 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD12 | 16 | 0.46 |
| (2,1752) | 1:142:A:LEU:HB3 | 1:142:A:LEU:HD13 | 16 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 3 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 6 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 7 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 9 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 10 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 13 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 17 | 0.46 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 19 | 0.46 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 20 | 0.46 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 14 | 0.46 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 3 | 0.46 |
| (2,82) | 1:77:A:LEU:H | 1:77:A:LEU:HB3 | 13 | 0.46 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 1 | 0.45 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 10 | 0.45 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 12 | 0.45 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 12 | 0.45 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 12 | 0.45 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 19 | 0.45 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 19 | 0.45 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 19 | 0.45 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 4 | 0.45 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 8 | 0.45 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 11 | 0.45 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 15 | 0.45 |
| (2,1030) | 1:179:A:ARG:HA | 1:179:A:ARG:HD2 | 18 | 0.45 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 12 | 0.45 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 11 | 0.45 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 2 | 0.44 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 3 | 0.44 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 9 | 0.44 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 8 | 0.44 |
| (2,82) | 1:77:A:LEU:H | 1:77:A:LEU:HB3 | 1 | 0.44 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 16 | 0.43 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 17 | 0.43 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 2 | 0.43 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 5 | 0.43 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 8 | 0.43 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 19 | 0.43 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 5 | 0.43 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 5 | 0.43 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 5 | 0.43 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 16 | 0.43 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 19 | 0.43 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 17 | 0.43 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 5 | 0.43 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 13 | 0.43 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 14 | 0.43 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 20 | 0.43 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 4 | 0.43 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 9 | 0.43 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 11 | 0.43 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 18 | 0.43 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 6 | 0.42 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 15 | 0.42 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 19 | 0.42 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 4 | 0.42 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 9 | 0.42 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 11 | 0.42 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 11 | 0.42 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 11 | 0.42 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 11 | 0.42 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 18 | 0.42 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 18 | 0.42 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 18 | 0.42 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 3 | 0.42 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 5 | 0.42 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 12 | 0.42 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 18 | 0.42 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 19 | 0.42 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 7 | 0.42 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 8 | 0.42 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 5 | 0.42 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 12 | 0.42 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 7 | 0.42 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 12 | 0.42 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 13 | 0.42 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 15 | 0.42 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 19 | 0.42 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 13 | 0.41 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 1 | 0.41 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 3 | 0.41 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 4 | 0.41 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 18 | 0.41 |
| (2,1262) | 1:103:A:THR:HA | 1:104:A:PRO:HD3 | 17 | 0.41 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 2 | 0.41 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 2 | 0.41 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 2 | 0.41 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 7 | 0.41 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 9 | 0.41 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 10 | 0.41 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 14 | 0.41 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 15 | 0.41 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 17 | 0.41 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 18 | 0.41 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 12 | 0.41 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 18 | 0.41 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 1 | 0.41 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 6 | 0.41 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 11 | 0.41 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 11 | 0.41 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 12 | 0.41 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 13 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 1 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 3 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 4 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 7 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 8 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 9 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 11 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 15 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 16 | 0.41 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 19 | 0.41 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 2 | 0.41 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 14 | 0.41 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 1 | 0.4 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 3 | 0.4 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 17 | 0.4 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 8 | 0.4 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 9 | 0.4 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 11 | 0.4 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 12 | 0.4 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 1 | 0.4 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 6 | 0.4 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 4 | 0.4 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 11 | 0.4 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 14 | 0.4 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 15 | 0.4 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 13 | 0.4 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 14 | 0.4 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 20 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 1 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 2 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 3 | 0.4 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 5 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 8 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 11 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 12 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 13 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 19 | 0.4 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 20 | 0.4 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 3 | 0.4 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 12 | 0.4 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 14 | 0.4 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 4 | 0.4 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 9 | 0.4 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 13 | 0.4 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 2 | 0.4 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 8 | 0.4 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 14 | 0.4 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 10 | 0.4 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 19 | 0.4 |
| (2,156) | 1:43:A:VAL:H | 1:43:A:VAL:HB | 18 | 0.4 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 6 | 0.4 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 17 | 0.4 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 10 | 0.39 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 9 | 0.39 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 14 | 0.39 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 15 | 0.39 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 1 | 0.39 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 3 | 0.39 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 17 | 0.39 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 18 | 0.39 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 19 | 0.39 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 16 | 0.39 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 6 | 0.39 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 5 | 0.39 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 8 | 0.39 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 6 | 0.39 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 6 | 0.39 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 6 | 0.39 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 10 | 0.39 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 10 | 0.39 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 10 | 0.39 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 6 | 0.39 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 5 | 0.39 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 9 | 0.39 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 17 | 0.39 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 20 | 0.39 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 7 | 0.39 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 13 | 0.39 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 15 | 0.39 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 16 | 0.39 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 2 | 0.39 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 16 | 0.39 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 20 | 0.39 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 2 | 0.39 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 10 | 0.39 |
| (2,154) | 1:82:A:ARG:HG3 | 1:83:A:GLU:H | 18 | 0.39 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 9 | 0.38 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 5 | 0.38 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 6 | 0.38 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 12 | 0.38 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 4 | 0.38 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 6 | 0.38 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 7 | 0.38 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 10 | 0.38 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 15 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 2 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 3 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 7 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 8 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 12 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 14 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 18 | 0.38 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 20 | 0.38 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 5 | 0.38 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 5 | 0.38 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 5 | 0.38 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 12 | 0.38 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 7 | 0.38 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 9 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 3 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 3 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 3 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 15 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 15 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 15 | 0.38 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 17 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 17 | 0.38 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 17 | 0.38 |
| (2,1029) | 1:129:A:GLN:HG2 | 1:130:A:ALA:HA | 4 | 0.38 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 8 | 0.38 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 10 | 0.38 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 20 | 0.38 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 5 | 0.38 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 6 | 0.38 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 6 | 0.38 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 4 | 0.37 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 19 | 0.37 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 7 | 0.37 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 8 | 0.37 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 10 | 0.37 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 11 | 0.37 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 13 | 0.37 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 2 | 0.37 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 14 | 0.37 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 20 | 0.37 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 4 | 0.37 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 5 | 0.37 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 9 | 0.37 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 10 | 0.37 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 11 | 0.37 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 13 | 0.37 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 17 | 0.37 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 1 | 0.37 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 1 | 0.37 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 1 | 0.37 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 10 | 0.37 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 10 | 0.37 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 10 | 0.37 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 7 | 0.37 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 16 | 0.37 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 17 | 0.37 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 16 | 0.37 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 11 | 0.37 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 12 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 4 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 4 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 4 | 0.37 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 7 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 7 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 7 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 16 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 16 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 16 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 20 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 20 | 0.37 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 20 | 0.37 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 1 | 0.37 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 6 | 0.37 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 11 | 0.37 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 1 | 0.37 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 20 | 0.37 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 5 | 0.36 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 6 | 0.36 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 12 | 0.36 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 18 | 0.36 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 2 | 0.36 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 16 | 0.36 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 19 | 0.36 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 20 | 0.36 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 5 | 0.36 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 15 | 0.36 |
| (2,1412) | 1:126:A:ALA:HA | 1:129:A:GLN:HB2 | 19 | 0.36 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 6 | 0.36 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 6 | 0.36 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 6 | 0.36 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 17 | 0.36 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 17 | 0.36 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 17 | 0.36 |
| (2,1293) | 1:110:A:ARG:HB2 | 1:110:A:ARG:HD3 | 5 | 0.36 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 14 | 0.36 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 20 | 0.36 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 9 | 0.36 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 9 | 0.36 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 9 | 0.36 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 2 | 0.36 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 15 | 0.36 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 19 | 0.36 |
| (2,833) | 1:106:A:TRP:H | 1:106:A:TRP:HB3 | 3 | 0.36 |
| (2,833) | 1:106:A:TRP:H | 1:106:A:TRP:HB3 | 12 | 0.36 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 6 | 0.36 |
| (2,498) | 1:48:A:GLU:H | 1:48:A:GLU:HB3 | 4 | 0.36 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 17 | 0.36 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 6 | 0.36 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 2 | 0.35 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 12 | 0.35 |
| (2,1415) | 1:126:A:ALA:H | 1:129:A:GLN:HB2 | 16 | 0.35 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 7 | 0.35 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 8 | 0.35 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 9 | 0.35 |
| (2,1267) | 1:37:A:PRO:HG2 | 1:134:A:PRO:HD3 | 10 | 0.35 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 8 | 0.35 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 8 | 0.35 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 8 | 0.35 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 7 | 0.35 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 13 | 0.35 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 16 | 0.35 |
| (2,833) | 1:106:A:TRP:H | 1:106:A:TRP:HB3 | 7 | 0.35 |
| (2,833) | 1:106:A:TRP:H | 1:106:A:TRP:HB3 | 16 | 0.35 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 8 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 2 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 3 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 7 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 8 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 14 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 15 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 17 | 0.35 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 20 | 0.35 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 8 | 0.35 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 13 | 0.35 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 20 | 0.35 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 13 | 0.34 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 11 | 0.34 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 14 | 0.34 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 20 | 0.34 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 20 | 0.34 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 20 | 0.34 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 2 | 0.34 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 6 | 0.34 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 12 | 0.34 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 14 | 0.34 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 16 | 0.34 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 20 | 0.34 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 6 | 0.34 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 6 | 0.34 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 6 | 0.34 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 10 | 0.34 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 5 | 0.34 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 9 | 0.34 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 5 | 0.34 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 10 | 0.34 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 3 | 0.34 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 10 | 0.34 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 3 | 0.34 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 9 | 0.34 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 17 | 0.34 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 15 | 0.34 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 20 | 0.33 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 4 | 0.33 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 1 | 0.33 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 5 | 0.33 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 11 | 0.33 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 15 | 0.33 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 18 | 0.33 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 7 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 1 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 1 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 1 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 3 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 3 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 3 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 4 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 4 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 4 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 5 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 5 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 5 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 7 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 7 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 7 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 8 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 8 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 8 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 9 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 9 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 9 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 10 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 10 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 10 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 11 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 11 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 11 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 12 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 12 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 12 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 13 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 13 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 13 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 14 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 14 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 14 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 15 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 15 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 15 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 16 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 16 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 16 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 17 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 17 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 17 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 18 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 18 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 18 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 19 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 19 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 19 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 20 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 20 | 0.33 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 20 | 0.33 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 4 | 0.33 |
| (2,833) | 1:106:A:TRP:H | 1:106:A:TRP:HB3 | 20 | 0.33 |
| (2,539) | 1:96:A:VAL:HB | 1:115:A:ALA:H | 16 | 0.33 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 1 | 0.33 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 2 | 0.33 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 6 | 0.33 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 11 | 0.33 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 18 | 0.33 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 20 | 0.33 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 1 | 0.33 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 4 | 0.33 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 6 | 0.33 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 13 | 0.33 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 3 | 0.33 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 5 | 0.33 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 10 | 0.33 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 1 | 0.33 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 16 | 0.32 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 1 | 0.32 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 6 | 0.32 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 9 | 0.32 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 13 | 0.32 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 19 | 0.32 |
| (2,1299) | 1:19:A:GLU:HB3 | 1:19:A:GLU:HG3 | 4 | 0.32 |
| (2,1299) | 1:19:A:GLU:HB3 | 1:19:A:GLU:HG3 | 15 | 0.32 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 4 | 0.32 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 5 | 0.32 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 6 | 0.32 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 12 | 0.32 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 13 | 0.32 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 17 | 0.32 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 1 | 0.32 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 11 | 0.32 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 16 | 0.32 |
| (2,132) | 1:131:A:TYR:HB2 | 1:133:A:LYS:H | 16 | 0.32 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 8 | 0.32 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 4 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 4 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 4 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 5 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 5 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 5 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 6 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 6 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 6 | 0.31 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 2 | 0.31 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 7 | 0.31 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 8 | 0.31 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 10 | 0.31 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 13 | 0.31 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 15 | 0.31 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 17 | 0.31 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 18 | 0.31 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 19 | 0.31 |
| (2,1524) | 1:50:A:LYS:HA | 1:50:A:LYS:HD3 | 18 | 0.31 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 4 | 0.31 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 9 | 0.31 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 17 | 0.31 |
| (2,1299) | 1:19:A:GLU:HB3 | 1:19:A:GLU:HG3 | 1 | 0.31 |
| (2,1299) | 1:19:A:GLU:HB3 | 1:19:A:GLU:HG3 | 5 | 0.31 |
| (2,1299) | 1:19:A:GLU:HB3 | 1:19:A:GLU:HG3 | 14 | 0.31 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 2 | 0.31 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 3 | 0.31 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 15 | 0.31 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 1 | 0.31 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 1 | 0.31 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 1 | 0.31 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 4 | 0.31 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 9 | 0.31 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 14 | 0.31 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 15 | 0.31 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 16 | 0.31 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 4 | 0.31 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 14 | 0.31 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 19 | 0.31 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 17 | 0.31 |
| (2,51) | 1:179:A:ARG:HG2 | 1:180:A:ASP:H | 12 | 0.31 |
| (2,29) | 1:179:A:ARG:H | 1:179:A:ARG:HD2 | 12 | 0.31 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 9 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 9 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 9 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 10 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 10 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 10 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 12 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 12 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 12 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG3 | 19 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG3 | 19 | 0.3 |
| (2,1853) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG3 | 19 | 0.3 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 14 | 0.3 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 15 | 0.3 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 3 | 0.3 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 4 | 0.3 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 16 | 0.3 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 16 | 0.3 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 16 | 0.3 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 16 | 0.3 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 3 | 0.3 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 8 | 0.3 |
| (2,1333) | 1:83:A:GLU:HB2 | 1:84:A:THR:HB | 10 | 0.3 |
| (2,1195) | 1:142:A:LEU:HA | 1:142:A:LEU:HD11 | 2 | 0.3 |
| (2,1195) | 1:142:A:LEU:HA | 1:142:A:LEU:HD12 | 2 | 0.3 |
| (2,1195) | 1:142:A:LEU:HA | 1:142:A:LEU:HD13 | 2 | 0.3 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 3 | 0.3 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 15 | 0.3 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 16 | 0.3 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 7 | 0.3 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 17 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 4 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 6 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 9 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 11 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 12 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 14 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 16 | 0.3 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 17 | 0.3 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 9 | 0.3 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 15 | 0.3 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 14 | 0.3 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 8 | 0.3 |
| (2,29) | 1:179:A:ARG:H | 1:179:A:ARG:HD2 | 1 | 0.3 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 1 | 0.3 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 6 | 0.3 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 9 | 0.3 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 10 | 0.3 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 1 | 0.29 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 7 | 0.29 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 8 | 0.29 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 11 | 0.29 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 20 | 0.29 |
| (2,1527) | 1:185:A:GLU:HA | 1:185:A:GLU:HG3 | 5 | 0.29 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 19 | 0.29 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 13 | 0.29 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 13 | 0.29 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 13 | 0.29 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG21 | 14 | 0.29 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG22 | 14 | 0.29 |
| (2,1160) | 1:77:A:LEU:HB2 | 1:78:A:THR:HG23 | 14 | 0.29 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 6 | 0.29 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 8 | 0.29 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 2 | 0.29 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 12 | 0.29 |
| (2,378) | 1:64:A:ASN:H | 1:134:A:PRO:HD2 | 19 | 0.29 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 5 | 0.29 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 7 | 0.29 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 10 | 0.29 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 15 | 0.29 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 19 | 0.29 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 1 | 0.29 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 2 | 0.29 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 12 | 0.29 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 16 | 0.29 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 17 | 0.29 |
| (2,29) | 1:179:A:ARG:H | 1:179:A:ARG:HD2 | 5 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 2 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 3 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 5 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 7 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 8 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 12 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 13 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 16 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 18 | 0.29 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 20 | 0.29 |
| (2,1281) | 1:16:A:VAL:H | 1:21:A:ARG:HD2 | 8 | 0.28 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 1 | 0.28 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 10 | 0.28 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 18 | 0.28 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 2 | 0.28 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 2 | 0.28 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 2 | 0.28 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 15 | 0.28 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 15 | 0.28 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 15 | 0.28 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 2 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 4 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 5 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 8 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 9 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 10 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 12 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 14 | 0.28 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 17 | 0.28 |
| (2,970) | 1:45:A:ARG:HA | 1:48:A:GLU:HB3 | 18 | 0.28 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 10 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG21 | 13 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG22 | 13 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG23 | 13 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG21 | 14 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG22 | 14 | 0.28 |
| (2,538) | 1:102:A:THR:H | 1:102:A:THR:HG23 | 14 | 0.28 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 5 | 0.28 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 3 | 0.28 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 5 | 0.28 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 3 | 0.28 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 11 | 0.28 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 18 | 0.28 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 20 | 0.28 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 11 | 0.28 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 17 | 0.28 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 19 | 0.28 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 7 | 0.28 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 10 | 0.28 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 3 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 2 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 2 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 2 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 7 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 7 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 7 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 12 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 12 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 12 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 15 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 15 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 15 | 0.27 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 18 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 18 | 0.27 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 18 | 0.27 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 10 | 0.27 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 10 | 0.27 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 10 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 7 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 7 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 7 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 18 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 18 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 18 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 20 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 20 | 0.27 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 20 | 0.27 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 11 | 0.27 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 18 | 0.27 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 19 | 0.27 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 13 | 0.27 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 17 | 0.27 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 1 | 0.27 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 16 | 0.27 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 4 | 0.27 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 2 | 0.27 |
| (2,238) | 1:170:A:GLY:HA3 | 1:171:A:GLY:H | 19 | 0.27 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 14 | 0.27 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 5 | 0.27 |
| (2,51) | 1:179:A:ARG:HG2 | 1:180:A:ASP:H | 5 | 0.27 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 4 | 0.27 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 14 | 0.27 |
| (2,1626) | 1:155:A:ARG:H | 1:157:A:GLN:HB3 | 17 | 0.26 |
| (2,1617) | 1:47:A:LEU:HA | 1:54:A:VAL:HB | 4 | 0.26 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 1 | 0.26 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 8 | 0.26 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 14 | 0.26 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 15 | 0.26 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 17 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 9 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 9 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 9 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 11 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 11 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 11 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 13 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 13 | 0.26 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 13 | 0.26 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 16 | 0.26 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 16 | 0.26 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 16 | 0.26 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 3 | 0.26 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 3 | 0.26 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 3 | 0.26 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 7 | 0.26 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 7 | 0.26 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 7 | 0.26 |
| (2,1151) | 1:107:A:LEU:HD21 | 1:108:A:THR:HA | 18 | 0.26 |
| (2,1151) | 1:107:A:LEU:HD22 | 1:108:A:THR:HA | 18 | 0.26 |
| (2,1151) | 1:107:A:LEU:HD23 | 1:108:A:THR:HA | 18 | 0.26 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 19 | 0.26 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 19 | 0.26 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 19 | 0.26 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 15 | 0.26 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 10 | 0.26 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 10 | 0.26 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 9 | 0.26 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 13 | 0.26 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 10 | 0.26 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 10 | 0.26 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 10 | 0.26 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 10 | 0.26 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 14 | 0.26 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 20 | 0.26 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 6 | 0.26 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 10 | 0.26 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 19 | 0.26 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 2 | 0.26 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 8 | 0.26 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 13 | 0.26 |
| (2,278) | 1:156:A:ALA:H | 1:157:A:GLN:HG3 | 8 | 0.26 |
| (2,238) | 1:170:A:GLY:HA3 | 1:171:A:GLY:H | 17 | 0.26 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD11 | 7 | 0.26 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD12 | 7 | 0.26 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD13 | 7 | 0.26 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD11 | 10 | 0.26 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD12 | 10 | 0.26 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD13 | 10 | 0.26 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 6 | 0.26 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 9 | 0.26 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 16 | 0.26 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 17 | 0.26 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 16 | 0.26 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 2 | 0.26 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 4 | 0.26 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 16 | 0.26 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 7 | 0.26 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 9 | 0.26 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 1 | 0.26 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 2 | 0.26 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 11 | 0.26 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 16 | 0.26 |
| (2,2) | 1:40:A:GLU:H | 1:40:A:GLU:HB2 | 15 | 0.26 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 6 | 0.26 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 16 | 0.26 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 20 | 0.26 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 3 | 0.25 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 6 | 0.25 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 9 | 0.25 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 11 | 0.25 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 12 | 0.25 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 4 | 0.25 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 4 | 0.25 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 4 | 0.25 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 8 | 0.25 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 8 | 0.25 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 8 | 0.25 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 20 | 0.25 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 20 | 0.25 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 20 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 5 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 5 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 5 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 9 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 9 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 9 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 10 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 10 | 0.25 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 10 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD21 | 1:108:A:THR:HA | 7 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD22 | 1:108:A:THR:HA | 7 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD23 | 1:108:A:THR:HA | 7 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD21 | 1:108:A:THR:HA | 10 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD22 | 1:108:A:THR:HA | 10 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD23 | 1:108:A:THR:HA | 10 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD21 | 1:108:A:THR:HA | 15 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD22 | 1:108:A:THR:HA | 15 | 0.25 |
| (2,1151) | 1:107:A:LEU:HD23 | 1:108:A:THR:HA | 15 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 1 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 1 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 1 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 3 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 3 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 3 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 6 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 6 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 6 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 9 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 9 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 9 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 10 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 10 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 10 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 12 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 12 | 0.25 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 12 | 0.25 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 20 | 0.25 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 20 | 0.25 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 2 | 0.25 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 4 | 0.25 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 7 | 0.25 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 8 | 0.25 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 13 | 0.25 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 9 | 0.25 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 3 | 0.25 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 4 | 0.25 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 10 | 0.25 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 12 | 0.25 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 20 | 0.25 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD11 | 2 | 0.25 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD12 | 2 | 0.25 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD13 | 2 | 0.25 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 3 | 0.25 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 4 | 0.25 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 13 | 0.25 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 10 | 0.25 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 20 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 5 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 6 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 8 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 10 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 12 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 13 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 17 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 18 | 0.25 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 20 | 0.25 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 15 | 0.25 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 4 | 0.25 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 13 | 0.25 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 3 | 0.25 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 14 | 0.25 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 11 | 0.25 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 1 | 0.25 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 5 | 0.24 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 14 | 0.24 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 14 | 0.24 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 14 | 0.24 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 19 | 0.24 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 19 | 0.24 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 19 | 0.24 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 3 | 0.24 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 3 | 0.24 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 3 | 0.24 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 13 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 13 | 0.24 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 13 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 11 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 11 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 11 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 13 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 13 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 13 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 14 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 14 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 14 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 17 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 17 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 17 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 20 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 20 | 0.24 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 20 | 0.24 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 5 | 0.24 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 5 | 0.24 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 5 | 0.24 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 19 | 0.24 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 19 | 0.24 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 19 | 0.24 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 15 | 0.24 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 15 | 0.24 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 15 | 0.24 |
| (2,1151) | 1:107:A:LEU:HD21 | 1:108:A:THR:HA | 2 | 0.24 |
| (2,1151) | 1:107:A:LEU:HD22 | 1:108:A:THR:HA | 2 | 0.24 |
| (2,1151) | 1:107:A:LEU:HD23 | 1:108:A:THR:HA | 2 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 2 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 2 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 2 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 4 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 4 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 4 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 11 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 11 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 11 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 14 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 14 | 0.24 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 14 | 0.24 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 7 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 16 | 0.24 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 17 | 0.24 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 1 | 0.24 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 18 | 0.24 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 19 | 0.24 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 4 | 0.24 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 15 | 0.24 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 1 | 0.24 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 15 | 0.24 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 12 | 0.24 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 1 | 0.24 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 8 | 0.24 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 12 | 0.24 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 17 | 0.24 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 18 | 0.24 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 20 | 0.24 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 4 | 0.24 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 18 | 0.24 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 20 | 0.24 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 6 | 0.24 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 15 | 0.24 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 18 | 0.24 |
| (2,238) | 1:170:A:GLY:HA3 | 1:171:A:GLY:H | 13 | 0.24 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 12 | 0.24 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 7 | 0.24 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 1 | 0.24 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 7 | 0.24 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 9 | 0.24 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 11 | 0.24 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 1 | 0.24 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 4 | 0.24 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 5 | 0.24 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 10 | 0.24 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 12 | 0.24 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 13 | 0.24 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 18 | 0.24 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 7 | 0.24 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 14 | 0.24 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 8 | 0.24 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 15 | 0.24 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 10 | 0.24 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 18 | 0.24 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 16 | 0.24 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 17 | 0.24 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 10 | 0.23 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 10 | 0.23 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 10 | 0.23 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 2 | 0.23 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 13 | 0.23 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 16 | 0.23 |
| (2,1583) | 1:46:A:LEU:HB3 | 1:48:A:GLU:H | 19 | 0.23 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 11 | 0.23 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 7 | 0.23 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 7 | 0.23 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 7 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 1 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 1 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 1 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 6 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 6 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 6 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 7 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 7 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 7 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 12 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 12 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 12 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 15 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 15 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 15 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 19 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 19 | 0.23 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 19 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 14 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 14 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 14 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 17 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 17 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 17 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 20 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 20 | 0.23 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 20 | 0.23 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 9 | 0.23 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 9 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 9 | 0.23 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 16 | 0.23 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 16 | 0.23 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 16 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 5 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 5 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 5 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 13 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 13 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 13 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 16 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 16 | 0.23 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 16 | 0.23 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 13 | 0.23 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 8 | 0.23 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 14 | 0.23 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 2 | 0.23 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 4 | 0.23 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 5 | 0.23 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 10 | 0.23 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 14 | 0.23 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 7 | 0.23 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 12 | 0.23 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 6 | 0.23 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 18 | 0.23 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 18 | 0.23 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 18 | 0.23 |
| (2,723) | 1:76:A:MET:HG3 | 1:77:A:LEU:H | 13 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 1 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 3 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 4 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 5 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 7 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 8 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 9 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 11 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 12 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 13 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 14 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 16 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 17 | 0.23 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 18 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 5 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 5 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 5 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 7 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 7 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 7 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 11 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 11 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 11 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 19 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 19 | 0.23 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 19 | 0.23 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 5 | 0.23 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 16 | 0.23 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 13 | 0.23 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 14 | 0.23 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 19 | 0.23 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 11 | 0.23 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 13 | 0.23 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 19 | 0.23 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 7 | 0.23 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 10 | 0.23 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 20 | 0.23 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 9 | 0.23 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 19 | 0.23 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 19 | 0.23 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 19 | 0.23 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 7 | 0.23 |
| (2,238) | 1:170:A:GLY:HA3 | 1:171:A:GLY:H | 8 | 0.23 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 5 | 0.23 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 1 | 0.23 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 5 | 0.23 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 17 | 0.23 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 18 | 0.23 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 20 | 0.23 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 15 | 0.23 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 2 | 0.23 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 6 | 0.23 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 8 | 0.23 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 9 | 0.23 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 17 | 0.23 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 19 | 0.23 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 20 | 0.23 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 2 | 0.23 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 5 | 0.23 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 12 | 0.23 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 17 | 0.23 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 20 | 0.23 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 13 | 0.23 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 7 | 0.23 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 10 | 0.23 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 19 | 0.23 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 20 | 0.23 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 2 | 0.22 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 2 | 0.22 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 2 | 0.22 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 20 | 0.22 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 20 | 0.22 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 20 | 0.22 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 7 | 0.22 |
| (2,1588) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG2 | 12 | 0.22 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 6 | 0.22 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 20 | 0.22 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 11 | 0.22 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 17 | 0.22 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 15 | 0.22 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 19 | 0.22 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 17 | 0.22 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 18 | 0.22 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 12 | 0.22 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 12 | 0.22 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 12 | 0.22 |
| (2,1270) | 1:67:A:GLN:HB2 | 1:70:A:PRO:HD3 | 11 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 2 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 2 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 2 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 4 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 4 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 4 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 8 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 8 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 8 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 16 | 0.22 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 16 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 16 | 0.22 |
| (2,1242) | 1:188:A:ARG:HG2 | 1:189:A:GLN:HA | 8 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 1 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 1 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 1 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 4 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 4 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 4 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 13 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 13 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 13 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 18 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 18 | 0.22 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 18 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 1 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 1 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 1 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 6 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 6 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 6 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 14 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 14 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 14 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 19 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 19 | 0.22 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 19 | 0.22 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 10 | 0.22 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 10 | 0.22 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 10 | 0.22 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 1 | 0.22 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 16 | 0.22 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 4 | 0.22 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 9 | 0.22 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 12 | 0.22 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 13 | 0.22 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 3 | 0.22 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 7 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 7 | 0.22 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 15 | 0.22 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 15 | 0.22 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 6 | 0.22 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 7 | 0.22 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 11 | 0.22 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 6 | 0.22 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 14 | 0.22 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 19 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 3 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 4 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 5 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 7 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 9 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 10 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 11 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 12 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 13 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 15 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 18 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 19 | 0.22 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 20 | 0.22 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 2 | 0.22 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 6 | 0.22 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 10 | 0.22 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 19 | 0.22 |
| (2,511) | 1:19:A:GLU:H | 1:19:A:GLU:HB3 | 20 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 2 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 2 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 2 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 6 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 6 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 6 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 8 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 8 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 8 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 9 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 9 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 9 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 14 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 14 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 14 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 15 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 15 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 15 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 20 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 20 | 0.22 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 20 | 0.22 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 9 | 0.22 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 11 | 0.22 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 6 | 0.22 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 7 | 0.22 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 15 | 0.22 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 2 | 0.22 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 3 | 0.22 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 16 | 0.22 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 13 | 0.22 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 14 | 0.22 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 18 | 0.22 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 8 | 0.22 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 6 | 0.22 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 6 | 0.22 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 6 | 0.22 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 2 | 0.22 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 8 | 0.22 |
| (2,238) | 1:170:A:GLY:HA3 | 1:171:A:GLY:H | 14 | 0.22 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 2 | 0.22 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 8 | 0.22 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 6 | 0.22 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 9 | 0.22 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 11 | 0.22 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 13 | 0.22 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 14 | 0.22 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 19 | 0.22 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 5 | 0.22 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 7 | 0.22 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 10 | 0.22 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 14 | 0.22 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 16 | 0.22 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 18 | 0.22 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 3 | 0.22 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 14 | 0.22 |
| (2,90) | 1:128:A:CYS:HB3 | 1:130:A:ALA:H | 19 | 0.22 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 3 | 0.22 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 7 | 0.22 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 14 | 0.22 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 8 | 0.22 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 8 | 0.22 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 8 | 0.22 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 3 | 0.22 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 14 | 0.22 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 3 | 0.22 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 14 | 0.22 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 15 | 0.22 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 7 | 0.21 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 7 | 0.21 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 7 | 0.21 |
| (2,1753) | 1:173:A:LEU:HD21 | 1:174:A:ASN:H | 11 | 0.21 |
| (2,1753) | 1:173:A:LEU:HD22 | 1:174:A:ASN:H | 11 | 0.21 |
| (2,1753) | 1:173:A:LEU:HD23 | 1:174:A:ASN:H | 11 | 0.21 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 10 | 0.21 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 20 | 0.21 |
| (2,1587) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG3 | 18 | 0.21 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 4 | 0.21 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 7 | 0.21 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 9 | 0.21 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 15 | 0.21 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 19 | 0.21 |
| (2,1523) | 1:172:A:ARG:H | 1:173:A:LEU:HA | 6 | 0.21 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 8 | 0.21 |
| (2,1381) | 1:130:A:ALA:HB1 | 1:131:A:TYR:HB3 | 3 | 0.21 |
| (2,1381) | 1:130:A:ALA:HB2 | 1:131:A:TYR:HB3 | 3 | 0.21 |
| (2,1381) | 1:130:A:ALA:HB3 | 1:131:A:TYR:HB3 | 3 | 0.21 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 10 | 0.21 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 13 | 0.21 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 4 | 0.21 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 4 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 4 | 0.21 |
| (2,1249) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HD2 | 18 | 0.21 |
| (2,1249) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HD2 | 18 | 0.21 |
| (2,1249) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HD2 | 18 | 0.21 |
| (2,1242) | 1:188:A:ARG:HG2 | 1:189:A:GLN:HA | 12 | 0.21 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 18 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 6 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 6 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 6 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 9 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 9 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 9 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 10 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 10 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 10 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 12 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 12 | 0.21 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 12 | 0.21 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 5 | 0.21 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 5 | 0.21 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 5 | 0.21 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 20 | 0.21 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 20 | 0.21 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 20 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 1 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 1 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 1 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 3 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 3 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 3 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 9 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 9 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 9 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 20 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 20 | 0.21 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 20 | 0.21 |
| (2,1110) | 1:84:A:THR:HA | 1:88:A:ARG:HB3 | 8 | 0.21 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 5 | 0.21 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 7 | 0.21 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 18 | 0.21 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 20 | 0.21 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 20 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 20 | 0.21 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 20 | 0.21 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 20 | 0.21 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 20 | 0.21 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 20 | 0.21 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 20 | 0.21 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 20 | 0.21 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 12 | 0.21 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 3 | 0.21 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 18 | 0.21 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 1 | 0.21 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 2 | 0.21 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 8 | 0.21 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 14 | 0.21 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 16 | 0.21 |
| (2,733) | 1:151:A:VAL:H | 1:151:A:VAL:HB | 17 | 0.21 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 13 | 0.21 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 13 | 0.21 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 13 | 0.21 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 19 | 0.21 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 19 | 0.21 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 19 | 0.21 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 4 | 0.21 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 6 | 0.21 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 11 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 1 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 1 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 1 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 3 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 3 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 3 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 12 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 12 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 12 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 13 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 13 | 0.21 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 13 | 0.21 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 12 | 0.21 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 17 | 0.21 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 5 | 0.21 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 9 | 0.21 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 11 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 1 | 0.21 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 5 | 0.21 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 12 | 0.21 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 14 | 0.21 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 17 | 0.21 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 3 | 0.21 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 11 | 0.21 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 2 | 0.21 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 7 | 0.21 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 20 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 1 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 1 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 1 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 10 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 10 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 10 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 12 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 12 | 0.21 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 12 | 0.21 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 15 | 0.21 |
| (2,206) | 1:47:A:LEU:HA | 1:50:A:LYS:H | 18 | 0.21 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 1 | 0.21 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 18 | 0.21 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 20 | 0.21 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 2 | 0.21 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 3 | 0.21 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 4 | 0.21 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 8 | 0.21 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 12 | 0.21 |
| (2,131) | 1:133:A:LYS:H | 1:133:A:LYS:HB3 | 15 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 1 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 3 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 4 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 11 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 12 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 13 | 0.21 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 15 | 0.21 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 11 | 0.21 |
| (2,89) | 1:129:A:GLN:HG2 | 1:130:A:ALA:H | 16 | 0.21 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 10 | 0.21 |
| (2,86) | 1:148:A:CYS:H | 1:153:A:GLU:HB2 | 20 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 4 | 0.21 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 4 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 4 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 6 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 6 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 6 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 16 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 16 | 0.21 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 16 | 0.21 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 6 | 0.21 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 15 | 0.21 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 3 | 0.21 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 4 | 0.21 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 18 | 0.21 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 19 | 0.21 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 4 | 0.21 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 8 | 0.21 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 6 | 0.21 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 8 | 0.21 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 11 | 0.21 |
| (2,1826) | 1:188:A:ARG:HG2 | 1:188:A:ARG:HD3 | 8 | 0.2 |
| (2,1826) | 1:188:A:ARG:HG2 | 1:188:A:ARG:HD3 | 11 | 0.2 |
| (2,1826) | 1:188:A:ARG:HG2 | 1:188:A:ARG:HD3 | 12 | 0.2 |
| (2,1826) | 1:188:A:ARG:HG2 | 1:188:A:ARG:HD3 | 15 | 0.2 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 13 | 0.2 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 13 | 0.2 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 13 | 0.2 |
| (2,1681) | 1:108:A:THR:HG21 | 1:109:A:GLY:HA2 | 20 | 0.2 |
| (2,1681) | 1:108:A:THR:HG22 | 1:109:A:GLY:HA2 | 20 | 0.2 |
| (2,1681) | 1:108:A:THR:HG23 | 1:109:A:GLY:HA2 | 20 | 0.2 |
| (2,1617) | 1:47:A:LEU:HA | 1:54:A:VAL:HB | 19 | 0.2 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 1 | 0.2 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 3 | 0.2 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 10 | 0.2 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 17 | 0.2 |
| (2,1523) | 1:172:A:ARG:H | 1:173:A:LEU:HA | 9 | 0.2 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 8 | 0.2 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 9 | 0.2 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 11 | 0.2 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 12 | 0.2 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 17 | 0.2 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 18 | 0.2 |
| (2,1275) | 1:16:A:VAL:HG11 | 1:21:A:ARG:HD2 | 12 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1275) | 1:16:A:VAL:HG12 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (2,1275) | 1:16:A:VAL:HG13 | 1:21:A:ARG:HD2 | 12 | 0.2 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 5 | 0.2 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 5 | 0.2 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 5 | 0.2 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 18 | 0.2 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 18 | 0.2 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 18 | 0.2 |
| (2,1242) | 1:188:A:ARG:HG2 | 1:189:A:GLN:HA | 11 | 0.2 |
| (2,1242) | 1:188:A:ARG:HG2 | 1:189:A:GLN:HA | 15 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 2 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 2 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 2 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 11 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 11 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 11 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 15 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 15 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 15 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 16 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 16 | 0.2 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 16 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 3 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 3 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 3 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 8 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 8 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 8 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 11 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 11 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 11 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 17 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 17 | 0.2 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 17 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 2 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 2 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 2 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 8 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 8 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 8 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 12 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 12 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 12 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 17 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 17 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 17 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 18 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 18 | 0.2 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 18 | 0.2 |
| (2,1090) | 1:26:A:PRO:HD2 | 1:165:A:VAL:HB | 3 | 0.2 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 3 | 0.2 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 6 | 0.2 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 1 | 0.2 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 7 | 0.2 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 12 | 0.2 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 19 | 0.2 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 2 | 0.2 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 5 | 0.2 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 6 | 0.2 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 11 | 0.2 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 5 | 0.2 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 19 | 0.2 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 5 | 0.2 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 7 | 0.2 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 13 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 4 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 4 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 4 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 16 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 16 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 16 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 17 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 17 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 17 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD11 | 18 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD12 | 18 | 0.2 |
| (2,509) | 1:58:A:LEU:H | 1:58:A:LEU:HD13 | 18 | 0.2 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 13 | 0.2 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 6 | 0.2 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 10 | 0.2 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 15 | 0.2 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 17 | 0.2 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 3 | 0.2 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 2 | 0.2 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 4 | 0.2 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 19 | 0.2 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 1 | 0.2 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 4 | 0.2 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 5 | 0.2 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 6 | 0.2 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 15 | 0.2 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 16 | 0.2 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 17 | 0.2 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 9 | 0.2 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 9 | 0.2 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 9 | 0.2 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 18 | 0.2 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 18 | 0.2 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 18 | 0.2 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 10 | 0.2 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD11 | 15 | 0.2 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD12 | 15 | 0.2 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD13 | 15 | 0.2 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 15 | 0.2 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 8 | 0.2 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 9 | 0.2 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 19 | 0.2 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 20 | 0.2 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 20 | 0.2 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 20 | 0.2 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 10 | 0.2 |
| (2,51) | 1:179:A:ARG:HG2 | 1:180:A:ASP:H | 14 | 0.2 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 1 | 0.2 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 16 | 0.2 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 9 | 0.2 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 17 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 3 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 3 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 3 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 4 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 4 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 4 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 14 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 14 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 14 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 16 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 16 | 0.19 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 16 | 0.19 |
| (2,1615) | 1:148:A:CYS:H | 1:149:A:ARG:HB3 | 9 | 0.19 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 12 | 0.19 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 13 | 0.19 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 18 | 0.19 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 1 | 0.19 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 7 | 0.19 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 14 | 0.19 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 5 | 0.19 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 6 | 0.19 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 14 | 0.19 |
| (2,1331) | 1:81:A:GLN:HG3 | 1:84:A:THR:HB | 14 | 0.19 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 6 | 0.19 |
| (2,1288) | 1:105:A:ARG:HB2 | 1:105:A:ARG:HD3 | 6 | 0.19 |
| (2,1288) | 1:105:A:ARG:HB2 | 1:105:A:ARG:HD3 | 11 | 0.19 |
| (2,1275) | 1:16:A:VAL:HG11 | 1:21:A:ARG:HD2 | 11 | 0.19 |
| (2,1275) | 1:16:A:VAL:HG12 | 1:21:A:ARG:HD2 | 11 | 0.19 |
| (2,1275) | 1:16:A:VAL:HG13 | 1:21:A:ARG:HD2 | 11 | 0.19 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 11 | 0.19 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 11 | 0.19 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 11 | 0.19 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 6 | 0.19 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 19 | 0.19 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 8 | 0.19 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 8 | 0.19 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 8 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 2 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 2 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 2 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 4 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 4 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 4 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 12 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 12 | 0.19 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 12 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 4 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 4 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 4 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 11 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 11 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 11 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 15 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 15 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 15 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 19 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 19 | 0.19 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 19 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD21 | 13 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD22 | 13 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD23 | 13 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD21 | 17 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD22 | 17 | 0.19 |
| (2,1201) | 1:173:A:LEU:HB3 | 1:173:A:LEU:HD23 | 17 | 0.19 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 8 | 0.19 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 8 | 0.19 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 8 | 0.19 |
| (2,1140) | 1:164:A:VAL:HG21 | 1:166:A:PRO:HB2 | 17 | 0.19 |
| (2,1140) | 1:164:A:VAL:HG22 | 1:166:A:PRO:HB2 | 17 | 0.19 |
| (2,1140) | 1:164:A:VAL:HG23 | 1:166:A:PRO:HB2 | 17 | 0.19 |
| (2,1109) | 1:177:A:GLU:HB3 | 1:178:A:ILE:HA | 18 | 0.19 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 4 | 0.19 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 4 | 0.19 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 4 | 0.19 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 1 | 0.19 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 11 | 0.19 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 15 | 0.19 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 17 | 0.19 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 19 | 0.19 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 4 | 0.19 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 9 | 0.19 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 14 | 0.19 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 17 | 0.19 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 4 | 0.19 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 7 | 0.19 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 8 | 0.19 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 9 | 0.19 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 12 | 0.19 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 3 | 0.19 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 3 | 0.19 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 3 | 0.19 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 3 | 0.19 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 3 | 0.19 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 3 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 3 | 0.19 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 3 | 0.19 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 3 | 0.19 |
| (2,878) | 1:74:A:ASP:H | 1:75:A:THR:HB | 8 | 0.19 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 9 | 0.19 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 2 | 0.19 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 8 | 0.19 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 9 | 0.19 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 15 | 0.19 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 4 | 0.19 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 4 | 0.19 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 4 | 0.19 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 5 | 0.19 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 5 | 0.19 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 5 | 0.19 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 20 | 0.19 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 20 | 0.19 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 20 | 0.19 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 3 | 0.19 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 8 | 0.19 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 15 | 0.19 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 18 | 0.19 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 19 | 0.19 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 20 | 0.19 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 6 | 0.19 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 19 | 0.19 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 11 | 0.19 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 9 | 0.19 |
| (2,402) | 1:184:A:GLY:H | 1:185:A:GLU:HB3 | 5 | 0.19 |
| (2,402) | 1:184:A:GLY:H | 1:185:A:GLU:HB3 | 9 | 0.19 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 9 | 0.19 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 10 | 0.19 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 11 | 0.19 |
| (2,366) | 1:171:A:GLY:H | 1:172:A:ARG:HB3 | 15 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 3 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 3 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 3 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 4 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 4 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 4 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 14 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 14 | 0.19 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 14 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 20 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 20 | 0.19 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 20 | 0.19 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 19 | 0.19 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 12 | 0.19 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 7 | 0.19 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 2 | 0.19 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 6 | 0.19 |
| (2,108) | 1:123:A:LEU:HB3 | 1:124:A:VAL:H | 17 | 0.19 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 9 | 0.19 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 9 | 0.19 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 9 | 0.19 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 17 | 0.19 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 17 | 0.19 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 17 | 0.19 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 5 | 0.19 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 12 | 0.19 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 19 | 0.19 |
| (2,51) | 1:179:A:ARG:HG2 | 1:180:A:ASP:H | 16 | 0.19 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 11 | 0.19 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 13 | 0.19 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 9 | 0.19 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 12 | 0.19 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 13 | 0.19 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 8 | 0.18 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 9 | 0.18 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 9 | 0.18 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 9 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG21 | 1:17:A:LEU:HD11 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG21 | 1:17:A:LEU:HD12 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG21 | 1:17:A:LEU:HD13 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG22 | 1:17:A:LEU:HD11 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG22 | 1:17:A:LEU:HD12 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG22 | 1:17:A:LEU:HD13 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG23 | 1:17:A:LEU:HD11 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG23 | 1:17:A:LEU:HD12 | 7 | 0.18 |
| (2,1767) | 1:14:A:ILE:HG23 | 1:17:A:LEU:HD13 | 7 | 0.18 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 11 | 0.18 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 11 | 0.18 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 11 | 0.18 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 4 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 2 | 0.18 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 5 | 0.18 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 14 | 0.18 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 9 | 0.18 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 19 | 0.18 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 1 | 0.18 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 4 | 0.18 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 7 | 0.18 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 15 | 0.18 |
| (2,1288) | 1:105:A:ARG:HB2 | 1:105:A:ARG:HD3 | 20 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG11 | 1:21:A:ARG:HD2 | 4 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG12 | 1:21:A:ARG:HD2 | 4 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG13 | 1:21:A:ARG:HD2 | 4 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG11 | 1:21:A:ARG:HD2 | 13 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG12 | 1:21:A:ARG:HD2 | 13 | 0.18 |
| (2,1275) | 1:16:A:VAL:HG13 | 1:21:A:ARG:HD2 | 13 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 8 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 8 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 8 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 13 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 13 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 13 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 14 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 14 | 0.18 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 14 | 0.18 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 16 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 7 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 7 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 7 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 10 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 10 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 10 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 16 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 16 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 16 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 18 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 18 | 0.18 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 18 | 0.18 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 3 | 0.18 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 3 | 0.18 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 3 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 5 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 5 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 5 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 6 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 6 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 6 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 13 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 13 | 0.18 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 13 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 2 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 2 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 2 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 7 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 7 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 7 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 20 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 20 | 0.18 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 20 | 0.18 |
| (2,1144) | 1:183:A:THR:HG21 | 1:185:A:GLU:HB3 | 6 | 0.18 |
| (2,1144) | 1:183:A:THR:HG22 | 1:185:A:GLU:HB3 | 6 | 0.18 |
| (2,1144) | 1:183:A:THR:HG23 | 1:185:A:GLU:HB3 | 6 | 0.18 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 11 | 0.18 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 13 | 0.18 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 15 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 3 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 3 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 3 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 5 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 5 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 5 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 10 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 10 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 10 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 20 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 20 | 0.18 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 20 | 0.18 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 6 | 0.18 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 2 | 0.18 |
| (2,1043) | 1:144:A:GLY:HA2 | 1:145:A:LEU:HA | 14 | 0.18 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 3 | 0.18 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 6 | 0.18 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 15 | 0.18 |
| (2,1023) | 1:179:A:ARG:HB2 | 1:181:A:ALA:HA | 14 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1023) | 1:179:A:ARG:HB2 | 1:181:A:ALA:HA | 16 | 0.18 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 1 | 0.18 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 10 | 0.18 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 13 | 0.18 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 20 | 0.18 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 4 | 0.18 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 11 | 0.18 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 11 | 0.18 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 2 | 0.18 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 4 | 0.18 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 15 | 0.18 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 5 | 0.18 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 5 | 0.18 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 5 | 0.18 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 8 | 0.18 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 8 | 0.18 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 8 | 0.18 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 13 | 0.18 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 13 | 0.18 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 13 | 0.18 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 12 | 0.18 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 12 | 0.18 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 12 | 0.18 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 3 | 0.18 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 10 | 0.18 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 17 | 0.18 |
| (2,720) | 1:104:A:PRO:HG2 | 1:105:A:ARG:H | 10 | 0.18 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 18 | 0.18 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 15 | 0.18 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 8 | 0.18 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 1 | 0.18 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 5 | 0.18 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 12 | 0.18 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 3 | 0.18 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 14 | 0.18 |
| (2,374) | 1:64:A:ASN:H | 1:128:A:CYS:HB2 | 19 | 0.18 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 13 | 0.18 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 13 | 0.18 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 13 | 0.18 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 16 | 0.18 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 16 | 0.18 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 16 | 0.18 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 8 | 0.18 |
| (2,322) | 1:113:A:SER:H | 1:114:A:LEU:HG | 1 | 0.18 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD11 | 18 | 0.18 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD12 | 18 | 0.18 |
| (2,200) | 1:106:A:TRP:H | 1:107:A:LEU:HD13 | 18 | 0.18 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 10 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 1 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 1 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 1 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 12 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 12 | 0.18 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 12 | 0.18 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 4 | 0.18 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 9 | 0.18 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 5 | 0.18 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 6 | 0.18 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 7 | 0.18 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 12 | 0.18 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 2 | 0.18 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 4 | 0.18 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 5 | 0.18 |
| (1,59) | 1:151:A:VAL:O | 1:155:A:ARG:H | 18 | 0.18 |
| (1,34) | 1:44:A:MET:O | 1:48:A:GLU:H | 18 | 0.18 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 4 | 0.17 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 12 | 0.17 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 13 | 0.17 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 16 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 1 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 1 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 1 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 5 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 5 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 5 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 6 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 6 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 6 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 11 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 11 | 0.17 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 11 | 0.17 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 5 | 0.17 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 5 | 0.17 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 5 | 0.17 |
| (2,1668) | 1:47:A:LEU:HB2 | 1:54:A:VAL:HG21 | 18 | 0.17 |
| (2,1668) | 1:47:A:LEU:HB2 | 1:54:A:VAL:HG22 | 18 | 0.17 |
| (2,1668) | 1:47:A:LEU:HB2 | 1:54:A:VAL:HG23 | 18 | 0.17 |
| (2,1599) | 1:10:A:ILE:HB | 1:11:A:ALA:HB1 | 17 | 0.17 |
| (2,1599) | 1:10:A:ILE:HB | 1:11:A:ALA:HB2 | 17 | 0.17 |
| (2,1599) | 1:10:A:ILE:HB | 1:11:A:ALA:HB3 | 17 | 0.17 |
| (2,1588) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG2 | 16 | 0.17 |
| (2,1587) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG3 | 19 | 0.17 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 8 | 0.17 |
| (2,1567) | 1:166:A:PRO:HB3 | 1:167:A:GLY:HA2 | 16 | 0.17 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 8 | 0.17 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 14 | 0.17 |
| (2,1478) | 1:30:A:VAL:HG11 | 1:31:A:PHE:HA | 10 | 0.17 |
| (2,1478) | 1:30:A:VAL:HG12 | 1:31:A:PHE:HA | 10 | 0.17 |
| (2,1478) | 1:30:A:VAL:HG13 | 1:31:A:PHE:HA | 10 | 0.17 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 2 | 0.17 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 2 | 0.17 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 6 | 0.17 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 15 | 0.17 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 2 | 0.17 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 3 | 0.17 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 16 | 0.17 |
| (2,1341) | 1:125:A:VAL:HA | 1:129:A:GLN:HG3 | 20 | 0.17 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 4 | 0.17 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 10 | 0.17 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 10 | 0.17 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 10 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 13 | 0.17 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 15 | 0.17 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 10 | 0.17 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 13 | 0.17 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 3 | 0.17 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 3 | 0.17 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 3 | 0.17 |
| (2,1218) | 1:49:A:LEU:HD21 | 1:51:A:GLN:HB3 | 13 | 0.17 |
| (2,1218) | 1:49:A:LEU:HD22 | 1:51:A:GLN:HB3 | 13 | 0.17 |
| (2,1218) | 1:49:A:LEU:HD23 | 1:51:A:GLN:HB3 | 13 | 0.17 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 7 | 0.17 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 17 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 9 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 9 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 9 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 12 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 12 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 12 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 16 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 16 | 0.17 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 16 | 0.17 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 9 | 0.17 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 19 | 0.17 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 5 | 0.17 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 11 | 0.17 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 13 | 0.17 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 16 | 0.17 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 18 | 0.17 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 15 | 0.17 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 16 | 0.17 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 6 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 12 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 16 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 16 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 18 | 0.17 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 18 | 0.17 |
| (2,900) | 1:83:A:GLU:HB2 | 1:87:A:SER:HB2 | 16 | 0.17 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 8 | 0.17 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 10 | 0.17 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 11 | 0.17 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 12 | 0.17 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 13 | 0.17 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 17 | 0.17 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 18 | 0.17 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 17 | 0.17 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 3 | 0.17 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 3 | 0.17 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 3 | 0.17 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 10 | 0.17 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 10 | 0.17 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 10 | 0.17 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 11 | 0.17 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 11 | 0.17 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 11 | 0.17 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 16 | 0.17 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 16 | 0.17 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 16 | 0.17 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 2 | 0.17 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 4 | 0.17 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 6 | 0.17 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 12 | 0.17 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 9 | 0.17 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 10 | 0.17 |
| (2,678) | 1:45:A:ARG:H | 1:45:A:ARG:HG2 | 20 | 0.17 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD21 | 11 | 0.17 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD22 | 11 | 0.17 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD23 | 11 | 0.17 |
| (2,497) | 1:48:A:GLU:H | 1:48:A:GLU:HG3 | 3 | 0.17 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 18 | 0.17 |
| (2,482) | 1:133:A:LYS:H | 1:134:A:PRO:HD3 | 16 | 0.17 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 7 | 0.17 |
| (2,432) | 1:37:A:PRO:HG3 | 1:38:A:ASP:H | 8 | 0.17 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 17 | 0.17 |
| (2,365) | 1:171:A:GLY:H | 1:172:A:ARG:HD2 | 7 | 0.17 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 17 | 0.17 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 17 | 0.17 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 17 | 0.17 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 9 | 0.17 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 14 | 0.17 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 12 | 0.17 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 12 | 0.17 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 12 | 0.17 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 13 | 0.17 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 13 | 0.17 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 13 | 0.17 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 11 | 0.17 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 19 | 0.17 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 19 | 0.17 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 19 | 0.17 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 9 | 0.17 |
| (2,5) | 1:39:A:SER:H | 1:40:A:GLU:H | 8 | 0.17 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 2 | 0.17 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 15 | 0.17 |
| (1,36) | 1:65:A:TYR:O | 1:69:A:LYS:H | 11 | 0.17 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 1 | 0.16 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 3 | 0.16 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 5 | 0.16 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 6 | 0.16 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 11 | 0.16 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 11 | 0.16 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 11 | 0.16 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 11 | 0.16 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 8 | 0.16 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 1 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 1 | 0.16 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 1 | 0.16 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 13 | 0.16 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 13 | 0.16 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 13 | 0.16 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 20 | 0.16 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 20 | 0.16 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 20 | 0.16 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 8 | 0.16 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 8 | 0.16 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 8 | 0.16 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 15 | 0.16 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 15 | 0.16 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 15 | 0.16 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 5 | 0.16 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 5 | 0.16 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 5 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD21 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD22 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD23 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD21 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD22 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD23 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD21 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD22 | 10 | 0.16 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD23 | 10 | 0.16 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 17 | 0.16 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 17 | 0.16 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 17 | 0.16 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 18 | 0.16 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 18 | 0.16 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 18 | 0.16 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 19 | 0.16 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 19 | 0.16 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 19 | 0.16 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 6 | 0.16 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 11 | 0.16 |
| (2,1615) | 1:148:A:CYS:H | 1:149:A:ARG:HB3 | 19 | 0.16 |
| (2,1588) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG2 | 4 | 0.16 |
| (2,1588) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG2 | 7 | 0.16 |
| (2,1588) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG2 | 17 | 0.16 |
| (2,1587) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG3 | 10 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 16 | 0.16 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 16 | 0.16 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 16 | 0.16 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 6 | 0.16 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 15 | 0.16 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 17 | 0.16 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 9 | 0.16 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 10 | 0.16 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 4 | 0.16 |
| (2,1316) | 1:6:A:GLN:HG2 | 1:7:A:ARG:H | 2 | 0.16 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 2 | 0.16 |
| (2,1275) | 1:16:A:VAL:HG11 | 1:21:A:ARG:HD2 | 15 | 0.16 |
| (2,1275) | 1:16:A:VAL:HG12 | 1:21:A:ARG:HD2 | 15 | 0.16 |
| (2,1275) | 1:16:A:VAL:HG13 | 1:21:A:ARG:HD2 | 15 | 0.16 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 9 | 0.16 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 9 | 0.16 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 9 | 0.16 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 1 | 0.16 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 6 | 0.16 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 2 | 0.16 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 4 | 0.16 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 5 | 0.16 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 18 | 0.16 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 20 | 0.16 |
| (2,1233) | 1:124:A:VAL:HG11 | 1:128:A:CYS:HB3 | 7 | 0.16 |
| (2,1233) | 1:124:A:VAL:HG12 | 1:128:A:CYS:HB3 | 7 | 0.16 |
| (2,1233) | 1:124:A:VAL:HG13 | 1:128:A:CYS:HB3 | 7 | 0.16 |
| (2,1204) | 1:124:A:VAL:HG21 | 1:126:A:ALA:H | 14 | 0.16 |
| (2,1204) | 1:124:A:VAL:HG22 | 1:126:A:ALA:H | 14 | 0.16 |
| (2,1204) | 1:124:A:VAL:HG23 | 1:126:A:ALA:H | 14 | 0.16 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 13 | 0.16 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 13 | 0.16 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 13 | 0.16 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 4 | 0.16 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 4 | 0.16 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 4 | 0.16 |
| (2,1144) | 1:183:A:THR:HG21 | 1:185:A:GLU:HB3 | 19 | 0.16 |
| (2,1144) | 1:183:A:THR:HG22 | 1:185:A:GLU:HB3 | 19 | 0.16 |
| (2,1144) | 1:183:A:THR:HG23 | 1:185:A:GLU:HB3 | 19 | 0.16 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 15 | 0.16 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 3 | 0.16 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 4 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 5 | 0.16 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 10 | 0.16 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 14 | 0.16 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 20 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 2 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 2 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 2 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 6 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 6 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 6 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 13 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 13 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 13 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 19 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 19 | 0.16 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 19 | 0.16 |
| (2,1073) | 1:115:A:ALA:H | 1:116:A:VAL:HB | 10 | 0.16 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 7 | 0.16 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 3 | 0.16 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 5 | 0.16 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 13 | 0.16 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 8 | 0.16 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 10 | 0.16 |
| (2,973) | 1:176:A:SER:HA | 1:177:A:GLU:HB3 | 16 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 1 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 8 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 8 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 9 | 0.16 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 9 | 0.16 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 5 | 0.16 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 5 | 0.16 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 5 | 0.16 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 6 | 0.16 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 6 | 0.16 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 6 | 0.16 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 6 | 0.16 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 16 | 0.16 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 11 | 0.16 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 6 | 0.16 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 6 | 0.16 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 6 | 0.16 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 7 | 0.16 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 7 | 0.16 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 7 | 0.16 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 9 | 0.16 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 9 | 0.16 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 9 | 0.16 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 12 | 0.16 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 12 | 0.16 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 12 | 0.16 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 17 | 0.16 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 17 | 0.16 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 17 | 0.16 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 18 | 0.16 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 18 | 0.16 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 18 | 0.16 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 1 | 0.16 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 1 | 0.16 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 1 | 0.16 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 7 | 0.16 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 7 | 0.16 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 7 | 0.16 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 9 | 0.16 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 9 | 0.16 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 9 | 0.16 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 10 | 0.16 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 10 | 0.16 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 10 | 0.16 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 17 | 0.16 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 17 | 0.16 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 17 | 0.16 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 9 | 0.16 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 11 | 0.16 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 13 | 0.16 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 15 | 0.16 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 13 | 0.16 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 17 | 0.16 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 15 | 0.16 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 19 | 0.16 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 9 | 0.16 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 13 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 5 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 5 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 5 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 7 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 7 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 7 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 11 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 11 | 0.16 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 11 | 0.16 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 12 | 0.16 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 15 | 0.16 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 17 | 0.16 |
| (2,263) | 1:177:A:GLU:H | 1:177:A:GLU:HB3 | 17 | 0.16 |
| (2,258) | 1:188:A:ARG:H | 1:188:A:ARG:HD3 | 13 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 4 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 4 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 4 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 16 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 16 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 16 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 19 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 19 | 0.16 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 19 | 0.16 |

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Continued from previous page...

| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,87) | 1:81:A:GLN:H | 1:81:A:GLN:HB3 | 13 | 0.16 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 7 | 0.16 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 7 | 0.16 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 7 | 0.16 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 8 | 0.16 |
| (1,91) | 1:97:A:PHE:H | 1:114:A:LEU:O | 1 | 0.16 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 17 | 0.16 |
| (1,36) | 1:65:A:TYR:O | 1:69:A:LYS:H | 19 | 0.16 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 7 | 0.15 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 9 | 0.15 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 10 | 0.15 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 14 | 0.15 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 18 | 0.15 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 15 | 0.15 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 15 | 0.15 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 15 | 0.15 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 16 | 0.15 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 16 | 0.15 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 16 | 0.15 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 15 | 0.15 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 11 | 0.15 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 11 | 0.15 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 11 | 0.15 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 12 | 0.15 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 12 | 0.15 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 12 | 0.15 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 6 | 0.15 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 6 | 0.15 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 6 | 0.15 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 20 | 0.15 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 20 | 0.15 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 20 | 0.15 |
| (2,1716) | 1:154:A:VAL:HG11 | 1:155:A:ARG:HB3 | 15 | 0.15 |
| (2,1716) | 1:154:A:VAL:HG12 | 1:155:A:ARG:HB3 | 15 | 0.15 |
| (2,1716) | 1:154:A:VAL:HG13 | 1:155:A:ARG:HB3 | 15 | 0.15 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 6 | 0.15 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 6 | 0.15 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 6 | 0.15 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 9 | 0.15 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 9 | 0.15 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 9 | 0.15 |
| (2,1681) | 1:108:A:THR:HG21 | 1:109:A:GLY:HA2 | 2 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1681) | 1:108:A:THR:HG22 | 1:109:A:GLY:HA2 | 2 | 0.15 |
| (2,1681) | 1:108:A:THR:HG23 | 1:109:A:GLY:HA2 | 2 | 0.15 |
| (2,1615) | 1:148:A:CYS:H | 1:149:A:ARG:HB3 | 15 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 3 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 3 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 3 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 4 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 4 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 4 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 8 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 8 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 8 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 11 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 11 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 11 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 12 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 12 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 12 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 13 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 13 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 13 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 14 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 14 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 14 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 17 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 17 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 17 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 19 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 19 | 0.15 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 19 | 0.15 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 5 | 0.15 |
| (2,1478) | 1:30:A:VAL:HG11 | 1:31:A:PHE:HA | 3 | 0.15 |
| (2,1478) | 1:30:A:VAL:HG12 | 1:31:A:PHE:HA | 3 | 0.15 |
| (2,1478) | 1:30:A:VAL:HG13 | 1:31:A:PHE:HA | 3 | 0.15 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 5 | 0.15 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 16 | 0.15 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 20 | 0.15 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 13 | 0.15 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 2 | 0.15 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 2 | 0.15 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 2 | 0.15 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 5 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|------------------|----------|---------------|
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 17 | 0.15 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 10 | 0.15 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 12 | 0.15 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 5 | 0.15 |
| (2,1281) | 1:16:A:VAL:H | 1:21:A:ARG:HD2 | 3 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 1 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 1 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 1 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 19 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 19 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 19 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 20 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 20 | 0.15 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 20 | 0.15 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 3 | 0.15 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 15 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 1 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 3 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 9 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 10 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 11 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 12 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 14 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 17 | 0.15 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 19 | 0.15 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 2 | 0.15 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 9 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 5 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 5 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 5 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 9 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 9 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 9 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 12 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 12 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 12 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 16 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 16 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 16 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 17 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 17 | 0.15 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 17 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 1 | 0.15 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 1 | 0.15 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 1 | 0.15 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 5 | 0.15 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 5 | 0.15 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 5 | 0.15 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 11 | 0.15 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 11 | 0.15 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 11 | 0.15 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 2 | 0.15 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 19 | 0.15 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 1 | 0.15 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 2 | 0.15 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 9 | 0.15 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 16 | 0.15 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 19 | 0.15 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 4 | 0.15 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 4 | 0.15 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 4 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 7 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 7 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 7 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 11 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 11 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 11 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 14 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 14 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 14 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 18 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 18 | 0.15 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 18 | 0.15 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 16 | 0.15 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 18 | 0.15 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 19 | 0.15 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 11 | 0.15 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 14 | 0.15 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 20 | 0.15 |
| (2,1031) | 1:141:A:ASN:HA | 1:142:A:LEU:HB3 | 20 | 0.15 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 17 | 0.15 |
| (2,930) | 1:62:A:ALA:HB1 | 1:68:A:LEU:H | 11 | 0.15 |
| (2,930) | 1:62:A:ALA:HB2 | 1:68:A:LEU:H | 11 | 0.15 |
| (2,930) | 1:62:A:ALA:HB3 | 1:68:A:LEU:H | 11 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,928) | 1:62:A:ALA:HB1 | 1:68:A:LEU:HA | 16 | 0.15 |
| (2,928) | 1:62:A:ALA:HB2 | 1:68:A:LEU:HA | 16 | 0.15 |
| (2,928) | 1:62:A:ALA:HB3 | 1:68:A:LEU:HA | 16 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 2 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 6 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 13 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 14 | 0.15 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 14 | 0.15 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 4 | 0.15 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 4 | 0.15 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 4 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 9 | 0.15 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 9 | 0.15 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 9 | 0.15 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 12 | 0.15 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 12 | 0.15 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 12 | 0.15 |
| (2,766) | 1:46:A:LEU:HG | 1:47:A:LEU:H | 10 | 0.15 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 1 | 0.15 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 3 | 0.15 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 7 | 0.15 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 1 | 0.15 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 1 | 0.15 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 1 | 0.15 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 4 | 0.15 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 4 | 0.15 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 4 | 0.15 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 11 | 0.15 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 11 | 0.15 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 11 | 0.15 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 15 | 0.15 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 15 | 0.15 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 15 | 0.15 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 19 | 0.15 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 19 | 0.15 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 19 | 0.15 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 20 | 0.15 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 20 | 0.15 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 20 | 0.15 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 8 | 0.15 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 8 | 0.15 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 8 | 0.15 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 5 | 0.15 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 7 | 0.15 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 14 | 0.15 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 18 | 0.15 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 20 | 0.15 |
| (2,723) | 1:76:A:MET:HG3 | 1:77:A:LEU:H | 1 | 0.15 |
| (2,720) | 1:104:A:PRO:HG2 | 1:105:A:ARG:H | 2 | 0.15 |
| (2,714) | 1:179:A:ARG:HD2 | 1:180:A:ASP:H | 7 | 0.15 |
| (2,660) | 1:105:A:ARG:H | 1:107:A:LEU:HG | 2 | 0.15 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD21 | 4 | 0.15 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD22 | 4 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD23 | 4 | 0.15 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD21 | 18 | 0.15 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD22 | 18 | 0.15 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD23 | 18 | 0.15 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 8 | 0.15 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 1 | 0.15 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 11 | 0.15 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 19 | 0.15 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 18 | 0.15 |
| (2,433) | 1:37:A:PRO:HG2 | 1:38:A:ASP:H | 6 | 0.15 |
| (2,433) | 1:37:A:PRO:HG2 | 1:38:A:ASP:H | 14 | 0.15 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 6 | 0.15 |
| (2,412) | 1:75:A:THR:H | 1:76:A:MET:HG3 | 15 | 0.15 |
| (2,385) | 1:35:A:CYS:H | 1:37:A:PRO:HD2 | 16 | 0.15 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 10 | 0.15 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 14 | 0.15 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 18 | 0.15 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 20 | 0.15 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 6 | 0.15 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 6 | 0.15 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 6 | 0.15 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 18 | 0.15 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 18 | 0.15 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 18 | 0.15 |
| (2,179) | 1:68:A:LEU:H | 1:71:A:TYR:HB3 | 19 | 0.15 |
| (2,144) | 1:78:A:THR:HG21 | 1:82:A:ARG:H | 16 | 0.15 |
| (2,144) | 1:78:A:THR:HG22 | 1:82:A:ARG:H | 16 | 0.15 |
| (2,144) | 1:78:A:THR:HG23 | 1:82:A:ARG:H | 16 | 0.15 |
| (2,124) | 1:17:A:LEU:HG | 1:18:A:ASN:H | 7 | 0.15 |
| (2,87) | 1:81:A:GLN:H | 1:81:A:GLN:HB3 | 20 | 0.15 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 15 | 0.15 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 15 | 0.15 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 15 | 0.15 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 1 | 0.15 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 8 | 0.15 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 13 | 0.15 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 14 | 0.15 |
| (2,51) | 1:179:A:ARG:HG2 | 1:180:A:ASP:H | 2 | 0.15 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 10 | 0.15 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 15 | 0.15 |
| (1,36) | 1:65:A:TYR:O | 1:69:A:LYS:H | 18 | 0.15 |
| (1,30) | 1:42:A:ALA:O | 1:46:A:LEU:H | 19 | 0.15 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 2 | 0.14 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 19 | 0.14 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 19 | 0.14 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 19 | 0.14 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 10 | 0.14 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 12 | 0.14 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 16 | 0.14 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 18 | 0.14 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 2 | 0.14 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 19 | 0.14 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 19 | 0.14 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 19 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 2 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 2 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 2 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 11 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 11 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 11 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 17 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 17 | 0.14 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 17 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD21 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD22 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD23 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD21 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD22 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD23 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD21 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD22 | 7 | 0.14 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD23 | 7 | 0.14 |
| (2,1715) | 1:154:A:VAL:HG11 | 1:164:A:VAL:HA | 3 | 0.14 |
| (2,1715) | 1:154:A:VAL:HG12 | 1:164:A:VAL:HA | 3 | 0.14 |
| (2,1715) | 1:154:A:VAL:HG13 | 1:164:A:VAL:HA | 3 | 0.14 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 2 | 0.14 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 2 | 0.14 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 2 | 0.14 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 10 | 0.14 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 10 | 0.14 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 10 | 0.14 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 12 | 0.14 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 12 | 0.14 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 15 | 0.14 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 15 | 0.14 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 15 | 0.14 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD21 | 10 | 0.14 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD22 | 10 | 0.14 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD23 | 10 | 0.14 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD21 | 15 | 0.14 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD22 | 15 | 0.14 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD23 | 15 | 0.14 |
| (2,1681) | 1:108:A:THR:HG21 | 1:109:A:GLY:HA2 | 11 | 0.14 |
| (2,1681) | 1:108:A:THR:HG22 | 1:109:A:GLY:HA2 | 11 | 0.14 |
| (2,1681) | 1:108:A:THR:HG23 | 1:109:A:GLY:HA2 | 11 | 0.14 |
| (2,1615) | 1:148:A:CYS:H | 1:149:A:ARG:HB3 | 6 | 0.14 |
| (2,1593) | 1:141:A:ASN:HB2 | 1:142:A:LEU:HB3 | 20 | 0.14 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 5 | 0.14 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 5 | 0.14 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 5 | 0.14 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 13 | 0.14 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 13 | 0.14 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 13 | 0.14 |
| (2,1519) | 1:19:A:GLU:HA | 1:21:A:ARG:HD3 | 8 | 0.14 |
| (2,1519) | 1:19:A:GLU:HA | 1:21:A:ARG:HD3 | 15 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 1 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 1 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 1 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 7 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 7 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 7 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 9 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 9 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 9 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 10 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 10 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 10 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 15 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 15 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 15 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 18 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 18 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 18 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD11 | 20 | 0.14 |
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD12 | 20 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1514) | 1:123:A:LEU:HA | 1:123:A:LEU:HD13 | 20 | 0.14 |
| (2,1495) | 1:81:A:GLN:HA | 1:81:A:GLN:HG3 | 14 | 0.14 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 12 | 0.14 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 15 | 0.14 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 3 | 0.14 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 8 | 0.14 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 19 | 0.14 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 12 | 0.14 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 5 | 0.14 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 19 | 0.14 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 9 | 0.14 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 15 | 0.14 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 15 | 0.14 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 15 | 0.14 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 17 | 0.14 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 17 | 0.14 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 17 | 0.14 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 2 | 0.14 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 10 | 0.14 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 11 | 0.14 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 13 | 0.14 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 18 | 0.14 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 7 | 0.14 |
| (2,1239) | 1:110:A:ARG:H | 1:110:A:ARG:HG2 | 8 | 0.14 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 3 | 0.14 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 3 | 0.14 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 3 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 4 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 4 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 4 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 5 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 5 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 5 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 8 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 8 | 0.14 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 8 | 0.14 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 3 | 0.14 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 3 | 0.14 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 3 | 0.14 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 8 | 0.14 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 8 | 0.14 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 8 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 14 | 0.14 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 14 | 0.14 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 14 | 0.14 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 15 | 0.14 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 15 | 0.14 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 15 | 0.14 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 3 | 0.14 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 3 | 0.14 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 3 | 0.14 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 16 | 0.14 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 16 | 0.14 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 16 | 0.14 |
| (2,1109) | 1:177:A:GLU:HB3 | 1:178:A:ILE:HA | 19 | 0.14 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 4 | 0.14 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 9 | 0.14 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 10 | 0.14 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 18 | 0.14 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 20 | 0.14 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 6 | 0.14 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 3 | 0.14 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 14 | 0.14 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 17 | 0.14 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 20 | 0.14 |
| (2,1095) | 1:52:A:ARG:HB3 | 1:53:A:PRO:HB3 | 8 | 0.14 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 2 | 0.14 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 2 | 0.14 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 2 | 0.14 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 8 | 0.14 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 8 | 0.14 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 8 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 1 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 1 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 1 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 8 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 8 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 8 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 15 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 15 | 0.14 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 15 | 0.14 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 20 | 0.14 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 4 | 0.14 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 14 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 20 | 0.14 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 10 | 0.14 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 2 | 0.14 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 17 | 0.14 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 12 | 0.14 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 19 | 0.14 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 20 | 0.14 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG21 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG22 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG23 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG21 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG22 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG23 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG21 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG22 | 8 | 0.14 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG23 | 8 | 0.14 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 19 | 0.14 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 19 | 0.14 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 10 | 0.14 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 10 | 0.14 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 10 | 0.14 |
| (2,907) | 1:156:A:ALA:HB1 | 1:157:A:GLN:HG2 | 19 | 0.14 |
| (2,907) | 1:156:A:ALA:HB2 | 1:157:A:GLN:HG2 | 19 | 0.14 |
| (2,907) | 1:156:A:ALA:HB3 | 1:157:A:GLN:HG2 | 19 | 0.14 |
| (2,766) | 1:46:A:LEU:HG | 1:47:A:LEU:H | 7 | 0.14 |
| (2,766) | 1:46:A:LEU:HG | 1:47:A:LEU:H | 16 | 0.14 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 14 | 0.14 |
| (2,735) | 1:151:A:VAL:H | 1:164:A:VAL:HB | 20 | 0.14 |
| (2,734) | 1:151:A:VAL:H | 1:153:A:GLU:HB3 | 10 | 0.14 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 2 | 0.14 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 2 | 0.14 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 2 | 0.14 |
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 14 | 0.14 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 14 | 0.14 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 14 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (2,732) | 1:136:A:VAL:HG11 | 1:137:A:SER:H | 16 | 0.14 |
| (2,732) | 1:136:A:VAL:HG12 | 1:137:A:SER:H | 16 | 0.14 |
| (2,732) | 1:136:A:VAL:HG13 | 1:137:A:SER:H | 16 | 0.14 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 2 | 0.14 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 2 | 0.14 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 2 | 0.14 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 3 | 0.14 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 3 | 0.14 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 3 | 0.14 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 6 | 0.14 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 6 | 0.14 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 6 | 0.14 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 14 | 0.14 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 14 | 0.14 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 14 | 0.14 |
| (2,730) | 1:58:A:LEU:HD21 | 1:137:A:SER:H | 15 | 0.14 |
| (2,730) | 1:58:A:LEU:HD22 | 1:137:A:SER:H | 15 | 0.14 |
| (2,730) | 1:58:A:LEU:HD23 | 1:137:A:SER:H | 15 | 0.14 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 1 | 0.14 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 19 | 0.14 |
| (2,720) | 1:104:A:PRO:HG2 | 1:105:A:ARG:H | 11 | 0.14 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD21 | 9 | 0.14 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD22 | 9 | 0.14 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD23 | 9 | 0.14 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD21 | 19 | 0.14 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD22 | 19 | 0.14 |
| (2,590) | 1:99:A:ALA:H | 1:114:A:LEU:HD23 | 19 | 0.14 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 20 | 0.14 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 2 | 0.14 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 6 | 0.14 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 2 | 0.14 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 9 | 0.14 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 18 | 0.14 |
| (2,412) | 1:75:A:THR:H | 1:76:A:MET:HG3 | 16 | 0.14 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 8 | 0.14 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 8 | 0.14 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 8 | 0.14 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 1 | 0.14 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 5 | 0.14 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 5 | 0.14 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 20 | 0.14 |
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 12 | 0.14 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 20 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 8 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 8 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 8 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 10 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 10 | 0.14 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 10 | 0.14 |
| (2,238) | 1:170:A:GLY:HA3 | 1:171:A:GLY:H | 11 | 0.14 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 12 | 0.14 |
| (2,170) | 1:173:A:LEU:HB2 | 1:174:A:ASN:H | 4 | 0.14 |
| (2,148) | 1:51:A:GLN:H | 1:51:A:GLN:HB3 | 9 | 0.14 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 11 | 0.14 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 13 | 0.14 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 20 | 0.14 |
| (1,78) | 1:35:A:CYS:H | 1:136:A:VAL:O | 19 | 0.14 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 10 | 0.14 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 17 | 0.14 |
| (1,30) | 1:42:A:ALA:O | 1:46:A:LEU:H | 1 | 0.14 |
| (1,30) | 1:42:A:ALA:O | 1:46:A:LEU:H | 6 | 0.14 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 19 | 0.13 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 2 | 0.13 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 4 | 0.13 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 7 | 0.13 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 11 | 0.13 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 20 | 0.13 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 10 | 0.13 |
| (2,1806) | 1:46:A:LEU:HD21 | 1:54:A:VAL:HA | 18 | 0.13 |
| (2,1806) | 1:46:A:LEU:HD22 | 1:54:A:VAL:HA | 18 | 0.13 |
| (2,1806) | 1:46:A:LEU:HD23 | 1:54:A:VAL:HA | 18 | 0.13 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 3 | 0.13 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 3 | 0.13 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 3 | 0.13 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 15 | 0.13 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 15 | 0.13 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 15 | 0.13 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 17 | 0.13 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 17 | 0.13 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 17 | 0.13 |
| (2,1771) | 1:17:A:LEU:HD11 | 1:18:A:ASN:HA | 3 | 0.13 |
| (2,1771) | 1:17:A:LEU:HD12 | 1:18:A:ASN:HA | 3 | 0.13 |
| (2,1771) | 1:17:A:LEU:HD13 | 1:18:A:ASN:HA | 3 | 0.13 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 11 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 11 | 0.13 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 11 | 0.13 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 15 | 0.13 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 15 | 0.13 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 15 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD21 | 1:187:A:PHE:HA | 2 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD22 | 1:187:A:PHE:HA | 2 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD23 | 1:187:A:PHE:HA | 2 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD21 | 1:187:A:PHE:HA | 16 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD22 | 1:187:A:PHE:HA | 16 | 0.13 |
| (2,1755) | 1:186:A:LEU:HD23 | 1:187:A:PHE:HA | 16 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 5 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 5 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 5 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 7 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 7 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 7 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 8 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 8 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 8 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 12 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 12 | 0.13 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 12 | 0.13 |
| (2,1715) | 1:154:A:VAL:HG11 | 1:164:A:VAL:HA | 16 | 0.13 |
| (2,1715) | 1:154:A:VAL:HG12 | 1:164:A:VAL:HA | 16 | 0.13 |
| (2,1715) | 1:154:A:VAL:HG13 | 1:164:A:VAL:HA | 16 | 0.13 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 4 | 0.13 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 4 | 0.13 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 4 | 0.13 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 10 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD21 | 2 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD22 | 2 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD23 | 2 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD21 | 7 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD22 | 7 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD23 | 7 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD21 | 18 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD22 | 18 | 0.13 |
| (2,1690) | 1:107:A:LEU:HB2 | 1:107:A:LEU:HD23 | 18 | 0.13 |
| (2,1683) | 1:118:A:VAL:HG11 | 1:120:A:ASP:HB3 | 5 | 0.13 |
| (2,1683) | 1:118:A:VAL:HG12 | 1:120:A:ASP:HB3 | 5 | 0.13 |
| (2,1683) | 1:118:A:VAL:HG13 | 1:120:A:ASP:HB3 | 5 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 15 | 0.13 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 19 | 0.13 |
| (2,1617) | 1:47:A:LEU:HA | 1:54:A:VAL:HB | 12 | 0.13 |
| (2,1617) | 1:47:A:LEU:HA | 1:54:A:VAL:HB | 17 | 0.13 |
| (2,1589) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HB3 | 3 | 0.13 |
| (2,1589) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HB3 | 15 | 0.13 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG21 | 2 | 0.13 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG22 | 2 | 0.13 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG23 | 2 | 0.13 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG21 | 20 | 0.13 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG22 | 20 | 0.13 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG23 | 20 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 7 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 7 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 7 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 8 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 8 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 8 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 10 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 10 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 10 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 11 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 11 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 11 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 18 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 18 | 0.13 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 18 | 0.13 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 3 | 0.13 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 6 | 0.13 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 16 | 0.13 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 19 | 0.13 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 6 | 0.13 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 7 | 0.13 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 10 | 0.13 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 19 | 0.13 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 18 | 0.13 |
| (2,1422) | 1:48:A:GLU:HB3 | 1:50:A:LYS:H | 18 | 0.13 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 7 | 0.13 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 7 | 0.13 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 7 | 0.13 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 4 | 0.13 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 6 | 0.13 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 8 | 0.13 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 9 | 0.13 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 11 | 0.13 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 13 | 0.13 |
| (2,1316) | 1:6:A:GLN:HG2 | 1:7:A:ARG:H | 15 | 0.13 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 5 | 0.13 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 6 | 0.13 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 7 | 0.13 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 12 | 0.13 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 1 | 0.13 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 13 | 0.13 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 14 | 0.13 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 4 | 0.13 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 10 | 0.13 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 4 | 0.13 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 7 | 0.13 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 17 | 0.13 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 20 | 0.13 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG11 | 10 | 0.13 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG12 | 10 | 0.13 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG13 | 10 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 2 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 2 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 2 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 11 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 11 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 11 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 15 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 15 | 0.13 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 15 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 10 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 10 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 10 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 11 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 11 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 11 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 13 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 13 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 13 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 15 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 15 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 15 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 17 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 17 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 17 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 18 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 18 | 0.13 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 18 | 0.13 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 9 | 0.13 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 9 | 0.13 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 9 | 0.13 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 13 | 0.13 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 13 | 0.13 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 13 | 0.13 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 19 | 0.13 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 19 | 0.13 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 19 | 0.13 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 2 | 0.13 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 2 | 0.13 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 2 | 0.13 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 9 | 0.13 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 9 | 0.13 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 9 | 0.13 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 6 | 0.13 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 6 | 0.13 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 6 | 0.13 |
| (2,1145) | 1:57:A:GLY:H | 1:108:A:THR:HG21 | 11 | 0.13 |
| (2,1145) | 1:57:A:GLY:H | 1:108:A:THR:HG22 | 11 | 0.13 |
| (2,1145) | 1:57:A:GLY:H | 1:108:A:THR:HG23 | 11 | 0.13 |
| (2,1110) | 1:84:A:THR:HA | 1:88:A:ARG:HB3 | 15 | 0.13 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 5 | 0.13 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 7 | 0.13 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 11 | 0.13 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 14 | 0.13 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 12 | 0.13 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 18 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 1 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 2 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 4 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 5 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 6 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 7 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 8 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 9 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 10 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 11 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 12 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 13 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 15 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 16 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 18 | 0.13 |
| (2,1096) | 1:149:A:ARG:HB3 | 1:149:A:ARG:HG3 | 19 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 5 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 5 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 5 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 9 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 9 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 9 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 13 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 13 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 13 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 16 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 16 | 0.13 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 16 | 0.13 |
| (2,1075) | 1:154:A:VAL:HG21 | 1:164:A:VAL:HB | 17 | 0.13 |
| (2,1075) | 1:154:A:VAL:HG22 | 1:164:A:VAL:HB | 17 | 0.13 |
| (2,1075) | 1:154:A:VAL:HG23 | 1:164:A:VAL:HB | 17 | 0.13 |
| (2,1073) | 1:115:A:ALA:H | 1:116:A:VAL:HB | 7 | 0.13 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 2 | 0.13 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 10 | 0.13 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 8 | 0.13 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 1 | 0.13 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 16 | 0.13 |
| (2,980) | 1:55:A:ASP:HB3 | 1:56:A:LYS:HA | 7 | 0.13 |
| (2,980) | 1:55:A:ASP:HB3 | 1:56:A:LYS:HA | 12 | 0.13 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 6 | 0.13 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 4 | 0.13 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 5 | 0.13 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 11 | 0.13 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 16 | 0.13 |
| (2,930) | 1:62:A:ALA:HB1 | 1:68:A:LEU:H | 18 | 0.13 |
| (2,930) | 1:62:A:ALA:HB2 | 1:68:A:LEU:H | 18 | 0.13 |
| (2,930) | 1:62:A:ALA:HB3 | 1:68:A:LEU:H | 18 | 0.13 |
| (2,928) | 1:62:A:ALA:HB1 | 1:68:A:LEU:HA | 14 | 0.13 |
| (2,928) | 1:62:A:ALA:HB2 | 1:68:A:LEU:HA | 14 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,928) | 1:62:A:ALA:HB3 | 1:68:A:LEU:HA | 14 | 0.13 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG21 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG22 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG23 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG21 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG22 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG23 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG21 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG22 | 1 | 0.13 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG23 | 1 | 0.13 |
| (2,909) | 1:42:A:ALA:HB1 | 1:45:A:ARG:HD3 | 3 | 0.13 |
| (2,909) | 1:42:A:ALA:HB2 | 1:45:A:ARG:HD3 | 3 | 0.13 |
| (2,909) | 1:42:A:ALA:HB3 | 1:45:A:ARG:HD3 | 3 | 0.13 |
| (2,909) | 1:42:A:ALA:HB1 | 1:45:A:ARG:HD3 | 17 | 0.13 |
| (2,909) | 1:42:A:ALA:HB2 | 1:45:A:ARG:HD3 | 17 | 0.13 |
| (2,909) | 1:42:A:ALA:HB3 | 1:45:A:ARG:HD3 | 17 | 0.13 |
| (2,845) | 1:105:A:ARG:HB2 | 1:109:A:GLY:H | 14 | 0.13 |
| (2,836) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 18 | 0.13 |
| (2,766) | 1:46:A:LEU:HG | 1:47:A:LEU:H | 13 | 0.13 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 16 | 0.13 |
| (2,722) | 1:75:A:THR:HG21 | 1:77:A:LEU:H | 8 | 0.13 |
| (2,722) | 1:75:A:THR:HG22 | 1:77:A:LEU:H | 8 | 0.13 |
| (2,722) | 1:75:A:THR:HG23 | 1:77:A:LEU:H | 8 | 0.13 |
| (2,720) | 1:104:A:PRO:HG2 | 1:105:A:ARG:H | 4 | 0.13 |
| (2,672) | 1:46:A:LEU:HA | 1:49:A:LEU:H | 18 | 0.13 |
| (2,660) | 1:105:A:ARG:H | 1:107:A:LEU:HG | 11 | 0.13 |
| (2,530) | 1:73:A:ASP:HB2 | 1:74:A:ASP:H | 12 | 0.13 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 7 | 0.13 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 11 | 0.13 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 11 | 0.13 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 14 | 0.13 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 5 | 0.13 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 7 | 0.13 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 20 | 0.13 |
| (2,383) | 1:158:A:PHE:HB2 | 1:159:A:GLY:H | 16 | 0.13 |
| (2,366) | 1:171:A:GLY:H | 1:172:A:ARG:HB3 | 16 | 0.13 |
| (2,365) | 1:171:A:GLY:H | 1:172:A:ARG:HD2 | 13 | 0.13 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 2 | 0.13 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 2 | 0.13 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 2 | 0.13 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 4 | 0.13 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 18 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 1 | 0.13 |
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 7 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 5 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 5 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 5 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 9 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 9 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 9 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 17 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 17 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 17 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 20 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 20 | 0.13 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 20 | 0.13 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 5 | 0.13 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 13 | 0.13 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 19 | 0.13 |
| (2,209) | 1:90:A:PRO:HD3 | 1:91:A:GLY:H | 9 | 0.13 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 4 | 0.13 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 9 | 0.13 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 2 | 0.13 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 2 | 0.13 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 2 | 0.13 |
| (2,165) | 1:176:A:SER:H | 1:177:A:GLU:HG3 | 12 | 0.13 |
| (2,165) | 1:176:A:SER:H | 1:177:A:GLU:HG3 | 15 | 0.13 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 10 | 0.13 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 10 | 0.13 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 10 | 0.13 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 13 | 0.13 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 13 | 0.13 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 13 | 0.13 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 10 | 0.13 |
| (2,67) | 1:47:A:LEU:HA | 1:52:A:ARG:H | 18 | 0.13 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 13 | 0.13 |
| (2,63) | 1:155:A:ARG:HB2 | 1:156:A:ALA:H | 18 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 2 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 3 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 4 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 6 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 7 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 9 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 11 | 0.13 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 17 | 0.13 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 19 | 0.13 |
| (1,90) | 1:97:A:PHE:N | 1:114:A:LEU:O | 10 | 0.13 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 4 | 0.13 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 5 | 0.13 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 6 | 0.13 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 20 | 0.13 |
| (1,34) | 1:44:A:MET:O | 1:48:A:GLU:H | 15 | 0.13 |
| (1,30) | 1:42:A:ALA:O | 1:46:A:LEU:H | 11 | 0.13 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 20 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 3 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 3 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 3 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 12 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 12 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 12 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 14 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 14 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 14 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 17 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 17 | 0.12 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 17 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD21 | 1 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD22 | 1 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD23 | 1 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD21 | 13 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD22 | 13 | 0.12 |
| (2,1860) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD23 | 13 | 0.12 |
| (2,1858) | 1:63:A:ALA:H | 1:67:A:GLN:HG2 | 18 | 0.12 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 3 | 0.12 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 6 | 0.12 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 13 | 0.12 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 7 | 0.12 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 13 | 0.12 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 16 | 0.12 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 12 | 0.12 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 12 | 0.12 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 12 | 0.12 |
| (2,1783) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HD2 | 17 | 0.12 |
| (2,1783) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HD2 | 17 | 0.12 |
| (2,1783) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HD2 | 17 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 2 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 2 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 10 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 10 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 10 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 13 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 13 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 13 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 14 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 14 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 14 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 18 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 18 | 0.12 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 18 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 4 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 4 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 4 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 15 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 15 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 15 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 18 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 18 | 0.12 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 18 | 0.12 |
| (2,1715) | 1:154:A:VAL:HG11 | 1:164:A:VAL:HA | 7 | 0.12 |
| (2,1715) | 1:154:A:VAL:HG12 | 1:164:A:VAL:HA | 7 | 0.12 |
| (2,1715) | 1:154:A:VAL:HG13 | 1:164:A:VAL:HA | 7 | 0.12 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 1 | 0.12 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 1 | 0.12 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 1 | 0.12 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 7 | 0.12 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 7 | 0.12 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 7 | 0.12 |
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 8 | 0.12 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 8 | 0.12 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 8 | 0.12 |
| (2,1698) | 1:78:A:THR:HG21 | 1:79:A:ASP:H | 13 | 0.12 |
| (2,1698) | 1:78:A:THR:HG22 | 1:79:A:ASP:H | 13 | 0.12 |
| (2,1698) | 1:78:A:THR:HG23 | 1:79:A:ASP:H | 13 | 0.12 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 2 | 0.12 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 7 | 0.12 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 18 | 0.12 |
| (2,1681) | 1:108:A:THR:HG21 | 1:109:A:GLY:HA2 | 8 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1681) | 1:108:A:THR:HG22 | 1:109:A:GLY:HA2 | 8 | 0.12 |
| (2,1681) | 1:108:A:THR:HG23 | 1:109:A:GLY:HA2 | 8 | 0.12 |
| (2,1681) | 1:108:A:THR:HG21 | 1:109:A:GLY:HA2 | 13 | 0.12 |
| (2,1681) | 1:108:A:THR:HG22 | 1:109:A:GLY:HA2 | 13 | 0.12 |
| (2,1681) | 1:108:A:THR:HG23 | 1:109:A:GLY:HA2 | 13 | 0.12 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 1 | 0.12 |
| (2,1588) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG2 | 5 | 0.12 |
| (2,1585) | 1:54:A:VAL:H | 1:55:A:ASP:HB3 | 15 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 2 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 2 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 2 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 4 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 4 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 4 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 6 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 6 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 6 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 9 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 9 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 9 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 19 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 19 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 19 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 20 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 20 | 0.12 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 20 | 0.12 |
| (2,1519) | 1:19:A:GLU:HA | 1:21:A:ARG:HD3 | 4 | 0.12 |
| (2,1502) | 1:79:A:ASP:HA | 1:82:A:ARG:HB2 | 5 | 0.12 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 20 | 0.12 |
| (2,1471) | 1:27:A:THR:HA | 1:28:A:GLU:HG2 | 6 | 0.12 |
| (2,1471) | 1:27:A:THR:HA | 1:28:A:GLU:HG2 | 14 | 0.12 |
| (2,1471) | 1:27:A:THR:HA | 1:28:A:GLU:HG2 | 16 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 2 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 8 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 9 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 10 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 11 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 14 | 0.12 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 17 | 0.12 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 13 | 0.12 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 18 | 0.12 |
| (2,1446) | 1:62:A:ALA:HA | 1:128:A:CYS:HB2 | 6 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1446) | 1:62:A:ALA:HA | 1:128:A:CYS:HB2 | 20 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 5 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 5 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 5 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 16 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 16 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 16 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 20 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 20 | 0.12 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 20 | 0.12 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 13 | 0.12 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 16 | 0.12 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 2 | 0.12 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 17 | 0.12 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 18 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 1 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 2 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 3 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 4 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 8 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 9 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 10 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 11 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 13 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 14 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 15 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 16 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 17 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 19 | 0.12 |
| (2,1306) | 1:177:A:GLU:HB3 | 1:177:A:GLU:HG3 | 20 | 0.12 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 7 | 0.12 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 12 | 0.12 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 17 | 0.12 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 19 | 0.12 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 20 | 0.12 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 1 | 0.12 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 2 | 0.12 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 6 | 0.12 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 14 | 0.12 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 20 | 0.12 |
| (2,1281) | 1:16:A:VAL:H | 1:21:A:ARG:HD2 | 6 | 0.12 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 2 | 0.12 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 2 | 0.12 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 7 | 0.12 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 7 | 0.12 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 7 | 0.12 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 5 | 0.12 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 9 | 0.12 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 14 | 0.12 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 19 | 0.12 |
| (2,1265) | 1:164:A:VAL:HB | 1:166:A:PRO:HD2 | 8 | 0.12 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD21 | 18 | 0.12 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD22 | 18 | 0.12 |
| (2,1256) | 1:45:A:ARG:HG2 | 1:46:A:LEU:HD23 | 18 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG11 | 8 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG12 | 8 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG13 | 8 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG11 | 15 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG12 | 15 | 0.12 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG13 | 15 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG11 | 1:135:A:LEU:HD21 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG11 | 1:135:A:LEU:HD22 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG11 | 1:135:A:LEU:HD23 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG12 | 1:135:A:LEU:HD21 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG12 | 1:135:A:LEU:HD22 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG12 | 1:135:A:LEU:HD23 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG13 | 1:135:A:LEU:HD21 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG13 | 1:135:A:LEU:HD22 | 16 | 0.12 |
| (2,1231) | 1:124:A:VAL:HG13 | 1:135:A:LEU:HD23 | 16 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 1 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 1 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 1 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 6 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 6 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 6 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 19 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 19 | 0.12 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 19 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 1 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 1 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 1 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 2 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 2 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 2 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 6 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 6 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 6 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 7 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 7 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 7 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 9 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 9 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 9 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 12 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 12 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 12 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 19 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 19 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 19 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 20 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 20 | 0.12 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 20 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 7 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 7 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 7 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 8 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 8 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 8 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 16 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 16 | 0.12 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 16 | 0.12 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 4 | 0.12 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 4 | 0.12 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 4 | 0.12 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 10 | 0.12 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 10 | 0.12 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 10 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD11 | 3 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD12 | 3 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD13 | 3 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD11 | 14 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD12 | 14 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD13 | 14 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD11 | 18 | 0.12 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD12 | 18 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD13 | 18 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 3 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 3 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 3 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 11 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 11 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 11 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 18 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 18 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 18 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 19 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 19 | 0.12 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 19 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 1 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 1 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 1 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 5 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 5 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 5 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 6 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 6 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 6 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 10 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 10 | 0.12 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 10 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 6 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 6 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 6 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 10 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 10 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 10 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 12 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 12 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 12 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 13 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 13 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 13 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 14 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 14 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 14 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 19 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 19 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 20 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 20 | 0.12 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 20 | 0.12 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 5 | 0.12 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 5 | 0.12 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 5 | 0.12 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 3 | 0.12 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 6 | 0.12 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 12 | 0.12 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 13 | 0.12 |
| (2,1105) | 1:151:A:VAL:HB | 1:167:A:GLY:H | 8 | 0.12 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 20 | 0.12 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 20 | 0.12 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 20 | 0.12 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 8 | 0.12 |
| (2,1064) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HE2 | 18 | 0.12 |
| (2,1064) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HE2 | 18 | 0.12 |
| (2,1064) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HE2 | 18 | 0.12 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 2 | 0.12 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 15 | 0.12 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 17 | 0.12 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 7 | 0.12 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 8 | 0.12 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 9 | 0.12 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 12 | 0.12 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD11 | 9 | 0.12 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD12 | 9 | 0.12 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD13 | 9 | 0.12 |
| (2,1009) | 1:55:A:ASP:HB2 | 1:110:A:ARG:HA | 1 | 0.12 |
| (2,1009) | 1:55:A:ASP:HB2 | 1:110:A:ARG:HA | 14 | 0.12 |
| (2,1009) | 1:55:A:ASP:HB2 | 1:110:A:ARG:HA | 15 | 0.12 |
| (2,980) | 1:55:A:ASP:HB3 | 1:56:A:LYS:HA | 17 | 0.12 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 3 | 0.12 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 9 | 0.12 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 12 | 0.12 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 13 | 0.12 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 14 | 0.12 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 15 | 0.12 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 9 | 0.12 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 13 | 0.12 |
| (2,930) | 1:62:A:ALA:HB1 | 1:68:A:LEU:H | 1 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,930) | 1:62:A:ALA:HB2 | 1:68:A:LEU:H | 1 | 0.12 |
| (2,930) | 1:62:A:ALA:HB3 | 1:68:A:LEU:H | 1 | 0.12 |
| (2,930) | 1:62:A:ALA:HB1 | 1:68:A:LEU:H | 10 | 0.12 |
| (2,930) | 1:62:A:ALA:HB2 | 1:68:A:LEU:H | 10 | 0.12 |
| (2,930) | 1:62:A:ALA:HB3 | 1:68:A:LEU:H | 10 | 0.12 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG21 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG22 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG23 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG21 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG22 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG23 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG21 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG22 | 20 | 0.12 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG23 | 20 | 0.12 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 5 | 0.12 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB1 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB2 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG21 | 1:181:A:ALA:HB3 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB1 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB2 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG22 | 1:181:A:ALA:HB3 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB1 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB2 | 17 | 0.12 |
| (2,917) | 1:96:A:VAL:HG23 | 1:181:A:ALA:HB3 | 17 | 0.12 |
| (2,909) | 1:42:A:ALA:HB1 | 1:45:A:ARG:HD3 | 8 | 0.12 |
| (2,909) | 1:42:A:ALA:HB2 | 1:45:A:ARG:HD3 | 8 | 0.12 |
| (2,909) | 1:42:A:ALA:HB3 | 1:45:A:ARG:HD3 | 8 | 0.12 |
| (2,909) | 1:42:A:ALA:HB1 | 1:45:A:ARG:HD3 | 12 | 0.12 |
| (2,909) | 1:42:A:ALA:HB2 | 1:45:A:ARG:HD3 | 12 | 0.12 |
| (2,909) | 1:42:A:ALA:HB3 | 1:45:A:ARG:HD3 | 12 | 0.12 |
| (2,845) | 1:105:A:ARG:HB2 | 1:109:A:GLY:H | 15 | 0.12 |
| (2,836) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 4 | 0.12 |
| (2,766) | 1:46:A:LEU:HG | 1:47:A:LEU:H | 2 | 0.12 |
| (2,720) | 1:104:A:PRO:HG2 | 1:105:A:ARG:H | 19 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,672) | 1:46:A:LEU:HA | 1:49:A:LEU:H | 13 | 0.12 |
| (2,660) | 1:105:A:ARG:H | 1:107:A:LEU:HG | 15 | 0.12 |
| (2,660) | 1:105:A:ARG:H | 1:107:A:LEU:HG | 16 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 7 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 7 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 7 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 10 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 10 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 10 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 14 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 14 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 14 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 15 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 15 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 15 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 16 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 16 | 0.12 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 16 | 0.12 |
| (2,611) | 1:163:A:PRO:HA | 1:164:A:VAL:H | 6 | 0.12 |
| (2,534) | 1:128:A:CYS:HB3 | 1:129:A:GLN:H | 4 | 0.12 |
| (2,530) | 1:73:A:ASP:HB2 | 1:74:A:ASP:H | 1 | 0.12 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 17 | 0.12 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 8 | 0.12 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 1 | 0.12 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 6 | 0.12 |
| (2,433) | 1:37:A:PRO:HG2 | 1:38:A:ASP:H | 1 | 0.12 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 1 | 0.12 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 11 | 0.12 |
| (2,412) | 1:75:A:THR:H | 1:76:A:MET:HG3 | 2 | 0.12 |
| (2,412) | 1:75:A:THR:H | 1:76:A:MET:HG3 | 14 | 0.12 |
| (2,366) | 1:171:A:GLY:H | 1:172:A:ARG:HB3 | 20 | 0.12 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG11 | 15 | 0.12 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG12 | 15 | 0.12 |
| (2,362) | 1:150:A:THR:H | 1:154:A:VAL:HG13 | 15 | 0.12 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 2 | 0.12 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 7 | 0.12 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 11 | 0.12 |
| (2,333) | 1:27:A:THR:H | 1:30:A:VAL:H | 14 | 0.12 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 2 | 0.12 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 7 | 0.12 |
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 18 | 0.12 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 3 | 0.12 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 3 | 0.12 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 3 | 0.12 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 2 | 0.12 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 17 | 0.12 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 5 | 0.12 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 6 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 3 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 3 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 3 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 7 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 7 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 7 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 14 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 14 | 0.12 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 14 | 0.12 |
| (2,101) | 1:151:A:VAL:H | 1:154:A:VAL:H | 15 | 0.12 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 3 | 0.12 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 4 | 0.12 |
| (2,61) | 1:60:A:LEU:HA | 1:117:A:ARG:H | 11 | 0.12 |
| (2,61) | 1:60:A:LEU:HA | 1:117:A:ARG:H | 15 | 0.12 |
| (2,39) | 1:103:A:THR:H | 1:104:A:PRO:HD2 | 20 | 0.12 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 1 | 0.12 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 1 | 0.12 |
| (1,37) | 1:67:A:GLN:O | 1:71:A:TYR:N | 12 | 0.12 |
| (1,37) | 1:67:A:GLN:O | 1:71:A:TYR:N | 14 | 0.12 |
| (1,30) | 1:42:A:ALA:O | 1:46:A:LEU:H | 15 | 0.12 |
| (1,20) | 1:13:A:ALA:O | 1:17:A:LEU:H | 4 | 0.12 |
| (1,20) | 1:13:A:ALA:O | 1:17:A:LEU:H | 11 | 0.12 |
| (1,20) | 1:13:A:ALA:O | 1:17:A:LEU:H | 15 | 0.12 |
| (2,1863) | 1:151:A:VAL:H | 1:166:A:PRO:HB3 | 15 | 0.11 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 2 | 0.11 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 2 | 0.11 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 2 | 0.11 |
| (2,1858) | 1:63:A:ALA:H | 1:67:A:GLN:HG2 | 9 | 0.11 |
| (2,1844) | 1:66:A:GLU:HB3 | 1:66:A:GLU:HG3 | 11 | 0.11 |
| (2,1831) | 1:105:A:ARG:HA | 1:105:A:ARG:HD2 | 5 | 0.11 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 17 | 0.11 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 19 | 0.11 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 5 | 0.11 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 6 | 0.11 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 19 | 0.11 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 20 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 4 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 4 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 4 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 6 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 6 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 6 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 7 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 7 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 7 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 8 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 8 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 8 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 17 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 17 | 0.11 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 17 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 10 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 10 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 10 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 13 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 13 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 13 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG21 | 1:35:A:CYS:HB3 | 14 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG22 | 1:35:A:CYS:HB3 | 14 | 0.11 |
| (2,1743) | 1:33:A:VAL:HG23 | 1:35:A:CYS:HB3 | 14 | 0.11 |
| (2,1734) | 1:150:A:THR:HG21 | 1:168:A:GLU:H | 8 | 0.11 |
| (2,1734) | 1:150:A:THR:HG22 | 1:168:A:GLU:H | 8 | 0.11 |
| (2,1734) | 1:150:A:THR:HG23 | 1:168:A:GLU:H | 8 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD21 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD22 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD23 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD21 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD22 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD23 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD21 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD22 | 11 | 0.11 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD23 | 11 | 0.11 |
| (2,1715) | 1:154:A:VAL:HG11 | 1:164:A:VAL:HA | 14 | 0.11 |
| (2,1715) | 1:154:A:VAL:HG12 | 1:164:A:VAL:HA | 14 | 0.11 |
| (2,1715) | 1:154:A:VAL:HG13 | 1:164:A:VAL:HA | 14 | 0.11 |
| (2,1702) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG3 | 6 | 0.11 |
| (2,1702) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG3 | 6 | 0.11 |
| (2,1702) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG3 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1701) | 1:78:A:THR:HG21 | 1:81:A:GLN:HG2 | 3 | 0.11 |
| (2,1701) | 1:78:A:THR:HG22 | 1:81:A:GLN:HG2 | 3 | 0.11 |
| (2,1701) | 1:78:A:THR:HG23 | 1:81:A:GLN:HG2 | 3 | 0.11 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 13 | 0.11 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 20 | 0.11 |
| (2,1681) | 1:108:A:THR:HG21 | 1:109:A:GLY:HA2 | 19 | 0.11 |
| (2,1681) | 1:108:A:THR:HG22 | 1:109:A:GLY:HA2 | 19 | 0.11 |
| (2,1681) | 1:108:A:THR:HG23 | 1:109:A:GLY:HA2 | 19 | 0.11 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 8 | 0.11 |
| (2,1617) | 1:47:A:LEU:HA | 1:54:A:VAL:HB | 18 | 0.11 |
| (2,1609) | 1:116:A:VAL:HG21 | 1:134:A:PRO:HB3 | 8 | 0.11 |
| (2,1609) | 1:116:A:VAL:HG22 | 1:134:A:PRO:HB3 | 8 | 0.11 |
| (2,1609) | 1:116:A:VAL:HG23 | 1:134:A:PRO:HB3 | 8 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG21 | 10 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG22 | 10 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG23 | 10 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG21 | 18 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG22 | 18 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG23 | 18 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG21 | 19 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG22 | 19 | 0.11 |
| (2,1572) | 1:57:A:GLY:HA3 | 1:108:A:THR:HG23 | 19 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 3 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 3 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 3 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 12 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 12 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 12 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 15 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 15 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 15 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 17 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 17 | 0.11 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 17 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG21 | 3 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG22 | 3 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG23 | 3 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG21 | 8 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG22 | 8 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG23 | 8 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG21 | 10 | 0.11 |
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG22 | 10 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1556) | 1:64:A:ASN:HA | 1:118:A:VAL:HG23 | 10 | 0.11 |
| (2,1519) | 1:19:A:GLU:HA | 1:21:A:ARG:HD3 | 13 | 0.11 |
| (2,1502) | 1:79:A:ASP:HA | 1:82:A:ARG:HB2 | 20 | 0.11 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 2 | 0.11 |
| (2,1494) | 1:47:A:LEU:HA | 1:54:A:VAL:HA | 9 | 0.11 |
| (2,1471) | 1:27:A:THR:HA | 1:28:A:GLU:HG2 | 10 | 0.11 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 1 | 0.11 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 3 | 0.11 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 4 | 0.11 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 19 | 0.11 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 4 | 0.11 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 9 | 0.11 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 12 | 0.11 |
| (2,1446) | 1:62:A:ALA:HA | 1:128:A:CYS:HB2 | 7 | 0.11 |
| (2,1441) | 1:111:A:PHE:H | 1:112:A:ASP:HA | 16 | 0.11 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 6 | 0.11 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 6 | 0.11 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 6 | 0.11 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 14 | 0.11 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 14 | 0.11 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 14 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG11 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG12 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG13 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG11 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG12 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG13 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG11 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG12 | 17 | 0.11 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG13 | 17 | 0.11 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 7 | 0.11 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 10 | 0.11 |
| (2,1345) | 1:43:A:VAL:HA | 1:47:A:LEU:HB2 | 13 | 0.11 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 3 | 0.11 |
| (2,1302) | 1:185:A:GLU:HB3 | 1:185:A:GLU:HG2 | 5 | 0.11 |
| (2,1302) | 1:185:A:GLU:HB3 | 1:185:A:GLU:HG2 | 9 | 0.11 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 8 | 0.11 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 9 | 0.11 |
| (2,1287) | 1:172:A:ARG:HA | 1:172:A:ARG:HD2 | 16 | 0.11 |
| (2,1281) | 1:16:A:VAL:H | 1:21:A:ARG:HD2 | 2 | 0.11 |
| (2,1281) | 1:16:A:VAL:H | 1:21:A:ARG:HD2 | 19 | 0.11 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG21 | 6 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG22 | 6 | 0.11 |
| (2,1273) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HG23 | 6 | 0.11 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 12 | 0.11 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 16 | 0.11 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG11 | 13 | 0.11 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG12 | 13 | 0.11 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG13 | 13 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 5 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 5 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 5 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 9 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 9 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 9 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 16 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 16 | 0.11 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 16 | 0.11 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 14 | 0.11 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 14 | 0.11 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 14 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 1 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 1 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 1 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 5 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 5 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 5 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 11 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 11 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 11 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 15 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 15 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 15 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 17 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 17 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 17 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 20 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 20 | 0.11 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 20 | 0.11 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 15 | 0.11 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 15 | 0.11 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 15 | 0.11 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD11 | 5 | 0.11 |
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD12 | 5 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1190) | 1:141:A:ASN:HA | 1:142:A:LEU:HD13 | 5 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 4 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 4 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 4 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 6 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 6 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 6 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 16 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 16 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 16 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 17 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 17 | 0.11 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 17 | 0.11 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 3 | 0.11 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 3 | 0.11 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 3 | 0.11 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 14 | 0.11 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 14 | 0.11 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 14 | 0.11 |
| (2,1183) | 1:22:A:VAL:HG21 | 1:138:A:THR:H | 10 | 0.11 |
| (2,1183) | 1:22:A:VAL:HG22 | 1:138:A:THR:H | 10 | 0.11 |
| (2,1183) | 1:22:A:VAL:HG23 | 1:138:A:THR:H | 10 | 0.11 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 16 | 0.11 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 16 | 0.11 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 16 | 0.11 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 18 | 0.11 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 18 | 0.11 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 18 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 1 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 1 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 1 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 12 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 12 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 12 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 13 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 13 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 13 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 14 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 14 | 0.11 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 14 | 0.11 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 1 | 0.11 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 17 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 10 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 10 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 10 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 11 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 11 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 11 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 17 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 17 | 0.11 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 17 | 0.11 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 12 | 0.11 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 17 | 0.11 |
| (2,1064) | 1:49:A:LEU:HD21 | 1:50:A:LYS:HE2 | 4 | 0.11 |
| (2,1064) | 1:49:A:LEU:HD22 | 1:50:A:LYS:HE2 | 4 | 0.11 |
| (2,1064) | 1:49:A:LEU:HD23 | 1:50:A:LYS:HE2 | 4 | 0.11 |
| (2,1055) | 1:72:A:ILE:HG21 | 1:73:A:ASP:HB2 | 7 | 0.11 |
| (2,1055) | 1:72:A:ILE:HG22 | 1:73:A:ASP:HB2 | 7 | 0.11 |
| (2,1055) | 1:72:A:ILE:HG23 | 1:73:A:ASP:HB2 | 7 | 0.11 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 9 | 0.11 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 12 | 0.11 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 5 | 0.11 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 19 | 0.11 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD21 | 2 | 0.11 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD22 | 2 | 0.11 |
| (2,1032) | 1:142:A:LEU:HA | 1:142:A:LEU:HD23 | 2 | 0.11 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD11 | 8 | 0.11 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD12 | 8 | 0.11 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD13 | 8 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HA | 3 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HA | 3 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HA | 3 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HA | 4 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HA | 4 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HA | 4 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HA | 9 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HA | 9 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HA | 9 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HA | 10 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HA | 10 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HA | 10 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD11 | 1:50:A:LYS:HA | 13 | 0.11 |
| (2,1012) | 1:49:A:LEU:HD12 | 1:50:A:LYS:HA | 13 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1012) | 1:49:A:LEU:HD13 | 1:50:A:LYS:HA | 13 | 0.11 |
| (2,1009) | 1:55:A:ASP:HB2 | 1:110:A:ARG:HA | 11 | 0.11 |
| (2,980) | 1:55:A:ASP:HB3 | 1:56:A:LYS:HA | 16 | 0.11 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 1 | 0.11 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 4 | 0.11 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 7 | 0.11 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 8 | 0.11 |
| (2,948) | 1:62:A:ALA:HA | 1:67:A:GLN:HG2 | 10 | 0.11 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 7 | 0.11 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 8 | 0.11 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 14 | 0.11 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 18 | 0.11 |
| (2,930) | 1:62:A:ALA:HB1 | 1:68:A:LEU:H | 19 | 0.11 |
| (2,930) | 1:62:A:ALA:HB2 | 1:68:A:LEU:H | 19 | 0.11 |
| (2,930) | 1:62:A:ALA:HB3 | 1:68:A:LEU:H | 19 | 0.11 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG21 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG22 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB1 | 1:154:A:VAL:HG23 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG21 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG22 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB2 | 1:154:A:VAL:HG23 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG21 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG22 | 7 | 0.11 |
| (2,920) | 1:24:A:ALA:HB3 | 1:154:A:VAL:HG23 | 7 | 0.11 |
| (2,868) | 1:73:A:ASP:HB2 | 1:75:A:THR:HB | 8 | 0.11 |
| (2,860) | 1:169:A:THR:HB | 1:171:A:GLY:H | 13 | 0.11 |
| (2,845) | 1:105:A:ARG:HB2 | 1:109:A:GLY:H | 2 | 0.11 |
| (2,836) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 2 | 0.11 |
| (2,836) | 1:50:A:LYS:H | 1:50:A:LYS:HD3 | 13 | 0.11 |
| (2,720) | 1:104:A:PRO:HG2 | 1:105:A:ARG:H | 8 | 0.11 |
| (2,672) | 1:46:A:LEU:HA | 1:49:A:LEU:H | 7 | 0.11 |
| (2,672) | 1:46:A:LEU:HA | 1:49:A:LEU:H | 16 | 0.11 |
| (2,672) | 1:46:A:LEU:HA | 1:49:A:LEU:H | 20 | 0.11 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 11 | 0.11 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 11 | 0.11 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 11 | 0.11 |
| (2,550) | 1:96:A:VAL:HG21 | 1:97:A:PHE:H | 12 | 0.11 |
| (2,550) | 1:96:A:VAL:HG22 | 1:97:A:PHE:H | 12 | 0.11 |
| (2,550) | 1:96:A:VAL:HG23 | 1:97:A:PHE:H | 12 | 0.11 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 15 | 0.11 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 7 | 0.11 |
| (2,494) | 1:154:A:VAL:H | 1:157:A:GLN:HB3 | 17 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|-----------------|----------|---------------|
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 5 | 0.11 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 9 | 0.11 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 12 | 0.11 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 17 | 0.11 |
| (2,472) | 1:69:A:LYS:H | 1:70:A:PRO:HG2 | 10 | 0.11 |
| (2,459) | 1:22:A:VAL:H | 1:45:A:ARG:HD2 | 20 | 0.11 |
| (2,435) | 1:38:A:ASP:H | 1:39:A:SER:H | 20 | 0.11 |
| (2,433) | 1:37:A:PRO:HG2 | 1:38:A:ASP:H | 9 | 0.11 |
| (2,433) | 1:37:A:PRO:HG2 | 1:38:A:ASP:H | 15 | 0.11 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 4 | 0.11 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 12 | 0.11 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 15 | 0.11 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 19 | 0.11 |
| (2,360) | 1:150:A:THR:H | 1:153:A:GLU:HG2 | 6 | 0.11 |
| (2,347) | 1:183:A:THR:H | 1:184:A:GLY:HA3 | 16 | 0.11 |
| (2,333) | 1:27:A:THR:H | 1:30:A:VAL:H | 16 | 0.11 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 9 | 0.11 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 10 | 0.11 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 12 | 0.11 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 13 | 0.11 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 15 | 0.11 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 16 | 0.11 |
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 2 | 0.11 |
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 4 | 0.11 |
| (2,299) | 1:88:A:ARG:H | 1:88:A:ARG:HD2 | 19 | 0.11 |
| (2,274) | 1:112:A:ASP:H | 1:112:A:ASP:HB3 | 8 | 0.11 |
| (2,274) | 1:112:A:ASP:H | 1:112:A:ASP:HB3 | 10 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 1 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 1 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 1 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 2 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 2 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 2 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 7 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 7 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 7 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD21 | 15 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD22 | 15 | 0.11 |
| (2,241) | 1:64:A:ASN:H | 1:68:A:LEU:HD23 | 15 | 0.11 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 3 | 0.11 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 6 | 0.11 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 8 | 0.11 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,209) | 1:90:A:PRO:HD3 | 1:91:A:GLY:H | 8 | 0.11 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 10 | 0.11 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 6 | 0.11 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 6 | 0.11 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 6 | 0.11 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 9 | 0.11 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 9 | 0.11 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 9 | 0.11 |
| (2,170) | 1:173:A:LEU:HB2 | 1:174:A:ASN:H | 9 | 0.11 |
| (2,155) | 1:50:A:LYS:HB3 | 1:51:A:GLN:H | 19 | 0.11 |
| (2,148) | 1:51:A:GLN:H | 1:51:A:GLN:HB3 | 1 | 0.11 |
| (2,148) | 1:51:A:GLN:H | 1:51:A:GLN:HB3 | 15 | 0.11 |
| (2,144) | 1:78:A:THR:HG21 | 1:82:A:ARG:H | 14 | 0.11 |
| (2,144) | 1:78:A:THR:HG22 | 1:82:A:ARG:H | 14 | 0.11 |
| (2,144) | 1:78:A:THR:HG23 | 1:82:A:ARG:H | 14 | 0.11 |
| (2,101) | 1:151:A:VAL:H | 1:154:A:VAL:H | 8 | 0.11 |
| (2,101) | 1:151:A:VAL:H | 1:154:A:VAL:H | 11 | 0.11 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 5 | 0.11 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 5 | 0.11 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 5 | 0.11 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 7 | 0.11 |
| (2,39) | 1:103:A:THR:H | 1:104:A:PRO:HD2 | 1 | 0.11 |
| (2,39) | 1:103:A:THR:H | 1:104:A:PRO:HD2 | 12 | 0.11 |
| (2,39) | 1:103:A:THR:H | 1:104:A:PRO:HD2 | 15 | 0.11 |
| (2,15) | 1:96:A:VAL:HB | 1:97:A:PHE:H | 7 | 0.11 |
| (2,10) | 1:24:A:ALA:H | 1:165:A:VAL:H | 15 | 0.11 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 14 | 0.11 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 18 | 0.11 |
| (1,90) | 1:97:A:PHE:N | 1:114:A:LEU:O | 7 | 0.11 |
| (1,90) | 1:97:A:PHE:N | 1:114:A:LEU:O | 18 | 0.11 |
| (1,84) | 1:61:A:ILE:H | 1:135:A:LEU:O | 6 | 0.11 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 3 | 0.11 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 15 | 0.11 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 18 | 0.11 |
| (1,49) | 1:123:A:LEU:O | 1:127:A:LEU:H | 16 | 0.11 |
| (1,37) | 1:67:A:GLN:O | 1:71:A:TYR:N | 10 | 0.11 |
| (1,36) | 1:65:A:TYR:O | 1:69:A:LYS:H | 2 | 0.11 |
| (1,36) | 1:65:A:TYR:O | 1:69:A:LYS:H | 5 | 0.11 |
| (1,20) | 1:13:A:ALA:O | 1:17:A:LEU:H | 7 | 0.11 |
| (1,20) | 1:13:A:ALA:O | 1:17:A:LEU:H | 8 | 0.11 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 4 | 0.1 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 4 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 4 | 0.1 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD11 | 8 | 0.1 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD12 | 8 | 0.1 |
| (2,1861) | 1:76:A:MET:HG2 | 1:77:A:LEU:HD13 | 8 | 0.1 |
| (2,1829) | 1:81:A:GLN:HG3 | 1:82:A:ARG:HD3 | 13 | 0.1 |
| (2,1824) | 1:19:A:GLU:H | 1:21:A:ARG:HD3 | 9 | 0.1 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 4 | 0.1 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 11 | 0.1 |
| (2,1813) | 1:52:A:ARG:HA | 1:53:A:PRO:HD2 | 12 | 0.1 |
| (2,1786) | 1:94:A:THR:HG21 | 1:115:A:ALA:H | 18 | 0.1 |
| (2,1786) | 1:94:A:THR:HG22 | 1:115:A:ALA:H | 18 | 0.1 |
| (2,1786) | 1:94:A:THR:HG23 | 1:115:A:ALA:H | 18 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD11 | 1:18:A:ASN:HA | 10 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD12 | 1:18:A:ASN:HA | 10 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD13 | 1:18:A:ASN:HA | 10 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD11 | 1:18:A:ASN:HA | 18 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD12 | 1:18:A:ASN:HA | 18 | 0.1 |
| (2,1771) | 1:17:A:LEU:HD13 | 1:18:A:ASN:HA | 18 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 3 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 3 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 3 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 9 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 9 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 9 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 12 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 12 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 12 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG11 | 1:161:A:ALA:H | 19 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG12 | 1:161:A:ALA:H | 19 | 0.1 |
| (2,1761) | 1:151:A:VAL:HG13 | 1:161:A:ALA:H | 19 | 0.1 |
| (2,1755) | 1:186:A:LEU:HD21 | 1:187:A:PHE:HA | 1 | 0.1 |
| (2,1755) | 1:186:A:LEU:HD22 | 1:187:A:PHE:HA | 1 | 0.1 |
| (2,1755) | 1:186:A:LEU:HD23 | 1:187:A:PHE:HA | 1 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD21 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD22 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD23 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD21 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD22 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD23 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD21 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD22 | 8 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD23 | 8 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD21 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD22 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD11 | 1:60:A:LEU:HD23 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD21 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD22 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD12 | 1:60:A:LEU:HD23 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD21 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD22 | 20 | 0.1 |
| (2,1729) | 1:58:A:LEU:HD13 | 1:60:A:LEU:HD23 | 20 | 0.1 |
| (2,1715) | 1:154:A:VAL:HG11 | 1:164:A:VAL:HA | 2 | 0.1 |
| (2,1715) | 1:154:A:VAL:HG12 | 1:164:A:VAL:HA | 2 | 0.1 |
| (2,1715) | 1:154:A:VAL:HG13 | 1:164:A:VAL:HA | 2 | 0.1 |
| (2,1695) | 1:50:A:LYS:HG3 | 1:53:A:PRO:HB3 | 16 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG11 | 1:120:A:ASP:HB3 | 2 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG12 | 1:120:A:ASP:HB3 | 2 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG13 | 1:120:A:ASP:HB3 | 2 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG11 | 1:120:A:ASP:HB3 | 3 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG12 | 1:120:A:ASP:HB3 | 3 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG13 | 1:120:A:ASP:HB3 | 3 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG11 | 1:120:A:ASP:HB3 | 4 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG12 | 1:120:A:ASP:HB3 | 4 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG13 | 1:120:A:ASP:HB3 | 4 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG11 | 1:120:A:ASP:HB3 | 6 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG12 | 1:120:A:ASP:HB3 | 6 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG13 | 1:120:A:ASP:HB3 | 6 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG11 | 1:120:A:ASP:HB3 | 19 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG12 | 1:120:A:ASP:HB3 | 19 | 0.1 |
| (2,1683) | 1:118:A:VAL:HG13 | 1:120:A:ASP:HB3 | 19 | 0.1 |
| (2,1622) | 1:48:A:GLU:H | 1:50:A:LYS:HB2 | 3 | 0.1 |
| (2,1617) | 1:47:A:LEU:HA | 1:54:A:VAL:HB | 5 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG21 | 1:134:A:PRO:HB3 | 6 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG22 | 1:134:A:PRO:HB3 | 6 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG23 | 1:134:A:PRO:HB3 | 6 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG21 | 1:134:A:PRO:HB3 | 15 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG22 | 1:134:A:PRO:HB3 | 15 | 0.1 |
| (2,1609) | 1:116:A:VAL:HG23 | 1:134:A:PRO:HB3 | 15 | 0.1 |
| (2,1587) | 1:55:A:ASP:HB3 | 1:110:A:ARG:HG3 | 2 | 0.1 |
| (2,1585) | 1:54:A:VAL:H | 1:55:A:ASP:HB3 | 3 | 0.1 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD11 | 16 | 0.1 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD12 | 16 | 0.1 |
| (2,1569) | 1:57:A:GLY:HA2 | 1:58:A:LEU:HD13 | 16 | 0.1 |
| (2,1519) | 1:19:A:GLU:HA | 1:21:A:ARG:HD3 | 12 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1471) | 1:27:A:THR:HA | 1:28:A:GLU:HG2 | 2 | 0.1 |
| (2,1471) | 1:27:A:THR:HA | 1:28:A:GLU:HG2 | 11 | 0.1 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 15 | 0.1 |
| (2,1458) | 1:82:A:ARG:HA | 1:82:A:ARG:HG3 | 18 | 0.1 |
| (2,1451) | 1:96:A:VAL:HB | 1:115:A:ALA:HA | 11 | 0.1 |
| (2,1446) | 1:62:A:ALA:HA | 1:128:A:CYS:HB2 | 16 | 0.1 |
| (2,1422) | 1:48:A:GLU:HB3 | 1:50:A:LYS:H | 2 | 0.1 |
| (2,1422) | 1:48:A:GLU:HB3 | 1:50:A:LYS:H | 4 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 1 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 1 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 1 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 10 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 10 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 10 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 17 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 17 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 17 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG21 | 1:19:A:GLU:HB3 | 18 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG22 | 1:19:A:GLU:HB3 | 18 | 0.1 |
| (2,1418) | 1:16:A:VAL:HG23 | 1:19:A:GLU:HB3 | 18 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG11 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG12 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG13 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG11 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG12 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG13 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG11 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG12 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG13 | 13 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG11 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG12 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG21 | 1:154:A:VAL:HG13 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG11 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG12 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG22 | 1:154:A:VAL:HG13 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG11 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG12 | 16 | 0.1 |
| (2,1390) | 1:151:A:VAL:HG23 | 1:154:A:VAL:HG13 | 16 | 0.1 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 8 | 0.1 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 11 | 0.1 |
| (2,1349) | 1:26:A:PRO:HD3 | 1:124:A:VAL:HA | 14 | 0.1 |
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 1 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (2,1325) | 1:160:A:ALA:H | 1:163:A:PRO:HG3 | 20 | 0.1 |
| (2,1300) | 1:15:A:ASP:H | 1:19:A:GLU:HG3 | 11 | 0.1 |
| (2,1283) | 1:188:A:ARG:HD3 | 1:189:A:GLN:HA | 11 | 0.1 |
| (2,1281) | 1:16:A:VAL:H | 1:21:A:ARG:HD2 | 16 | 0.1 |
| (2,1269) | 1:67:A:GLN:HG2 | 1:70:A:PRO:HD3 | 8 | 0.1 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG11 | 12 | 0.1 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG12 | 12 | 0.1 |
| (2,1235) | 1:118:A:VAL:HA | 1:124:A:VAL:HG13 | 12 | 0.1 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG11 | 18 | 0.1 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG12 | 18 | 0.1 |
| (2,1228) | 1:61:A:ILE:HB | 1:124:A:VAL:HG13 | 18 | 0.1 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG21 | 16 | 0.1 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG22 | 16 | 0.1 |
| (2,1207) | 1:122:A:PRO:HD3 | 1:124:A:VAL:HG23 | 16 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 3 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 3 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 3 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 10 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 10 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 10 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 14 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 14 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 14 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG11 | 1:162:A:PHE:H | 19 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG12 | 1:162:A:PHE:H | 19 | 0.1 |
| (2,1205) | 1:151:A:VAL:HG13 | 1:162:A:PHE:H | 19 | 0.1 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD11 | 11 | 0.1 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD12 | 11 | 0.1 |
| (2,1197) | 1:44:A:MET:H | 1:47:A:LEU:HD13 | 11 | 0.1 |
| (2,1189) | 1:16:A:VAL:HG21 | 1:34:A:GLY:H | 12 | 0.1 |
| (2,1189) | 1:16:A:VAL:HG22 | 1:34:A:GLY:H | 12 | 0.1 |
| (2,1189) | 1:16:A:VAL:HG23 | 1:34:A:GLY:H | 12 | 0.1 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG21 | 9 | 0.1 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG22 | 9 | 0.1 |
| (2,1184) | 1:22:A:VAL:H | 1:22:A:VAL:HG23 | 9 | 0.1 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 7 | 0.1 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 7 | 0.1 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 7 | 0.1 |
| (2,1165) | 1:154:A:VAL:HG11 | 1:159:A:GLY:HA2 | 11 | 0.1 |
| (2,1165) | 1:154:A:VAL:HG12 | 1:159:A:GLY:HA2 | 11 | 0.1 |
| (2,1165) | 1:154:A:VAL:HG13 | 1:159:A:GLY:HA2 | 11 | 0.1 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG11 | 15 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG12 | 15 | 0.1 |
| (2,1147) | 1:64:A:ASN:HA | 1:118:A:VAL:HG13 | 15 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD11 | 1:99:A:ALA:HB1 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD11 | 1:99:A:ALA:HB2 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD11 | 1:99:A:ALA:HB3 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD12 | 1:99:A:ALA:HB1 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD12 | 1:99:A:ALA:HB2 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD12 | 1:99:A:ALA:HB3 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD13 | 1:99:A:ALA:HB1 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD13 | 1:99:A:ALA:HB2 | 9 | 0.1 |
| (2,1115) | 1:72:A:ILE:HD13 | 1:99:A:ALA:HB3 | 9 | 0.1 |
| (2,1110) | 1:84:A:THR:HA | 1:88:A:ARG:HB3 | 9 | 0.1 |
| (2,1107) | 1:151:A:VAL:HB | 1:166:A:PRO:HA | 16 | 0.1 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 18 | 0.1 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 18 | 0.1 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 18 | 0.1 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG21 | 19 | 0.1 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG22 | 19 | 0.1 |
| (2,1084) | 1:59:A:ILE:HB | 1:94:A:THR:HG23 | 19 | 0.1 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 5 | 0.1 |
| (2,1071) | 1:23:A:ILE:H | 1:25:A:TYR:HB2 | 18 | 0.1 |
| (2,1049) | 1:68:A:LEU:HB3 | 1:71:A:TYR:H | 7 | 0.1 |
| (2,1038) | 1:34:A:GLY:HA2 | 1:136:A:VAL:HB | 6 | 0.1 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD11 | 14 | 0.1 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD12 | 14 | 0.1 |
| (2,1028) | 1:12:A:ALA:HA | 1:23:A:ILE:HD13 | 14 | 0.1 |
| (2,1009) | 1:55:A:ASP:HB2 | 1:110:A:ARG:HA | 6 | 0.1 |
| (2,998) | 1:66:A:GLU:HB2 | 1:67:A:GLN:HA | 11 | 0.1 |
| (2,980) | 1:55:A:ASP:HB3 | 1:56:A:LYS:HA | 19 | 0.1 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 1 | 0.1 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 2 | 0.1 |
| (2,937) | 1:81:A:GLN:HB3 | 1:82:A:ARG:HD2 | 10 | 0.1 |
| (2,930) | 1:62:A:ALA:HB1 | 1:68:A:LEU:H | 5 | 0.1 |
| (2,930) | 1:62:A:ALA:HB2 | 1:68:A:LEU:H | 5 | 0.1 |
| (2,930) | 1:62:A:ALA:HB3 | 1:68:A:LEU:H | 5 | 0.1 |
| (2,766) | 1:46:A:LEU:HG | 1:47:A:LEU:H | 20 | 0.1 |
| (2,729) | 1:60:A:LEU:HB2 | 1:137:A:SER:H | 8 | 0.1 |
| (2,672) | 1:46:A:LEU:HA | 1:49:A:LEU:H | 10 | 0.1 |
| (2,660) | 1:105:A:ARG:H | 1:107:A:LEU:HG | 7 | 0.1 |
| (2,660) | 1:105:A:ARG:H | 1:107:A:LEU:HG | 12 | 0.1 |
| (2,637) | 1:145:A:LEU:H | 1:145:A:LEU:HB3 | 20 | 0.1 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG21 | 20 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|---------|-----------------|------------------|----------|---------------|
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG22 | 20 | 0.1 |
| (2,626) | 1:61:A:ILE:H | 1:136:A:VAL:HG23 | 20 | 0.1 |
| (2,611) | 1:163:A:PRO:HA | 1:164:A:VAL:H | 3 | 0.1 |
| (2,530) | 1:73:A:ASP:HB2 | 1:74:A:ASP:H | 17 | 0.1 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 2 | 0.1 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 3 | 0.1 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 8 | 0.1 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 14 | 0.1 |
| (2,496) | 1:154:A:VAL:H | 1:157:A:GLN:HG2 | 16 | 0.1 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 3 | 0.1 |
| (2,491) | 1:48:A:GLU:H | 1:49:A:LEU:H | 14 | 0.1 |
| (2,423) | 1:87:A:SER:H | 1:88:A:ARG:HB3 | 2 | 0.1 |
| (2,383) | 1:158:A:PHE:HB2 | 1:159:A:GLY:H | 15 | 0.1 |
| (2,333) | 1:27:A:THR:H | 1:30:A:VAL:H | 1 | 0.1 |
| (2,333) | 1:27:A:THR:H | 1:30:A:VAL:H | 15 | 0.1 |
| (2,309) | 1:21:A:ARG:HD2 | 1:22:A:VAL:H | 13 | 0.1 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 1 | 0.1 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 3 | 0.1 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 4 | 0.1 |
| (2,303) | 1:122:A:PRO:HD3 | 1:125:A:VAL:H | 11 | 0.1 |
| (2,275) | 1:105:A:ARG:H | 1:105:A:ARG:HD3 | 4 | 0.1 |
| (2,226) | 1:168:A:GLU:HB3 | 1:169:A:THR:H | 9 | 0.1 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 7 | 0.1 |
| (2,215) | 1:70:A:PRO:HG2 | 1:71:A:TYR:H | 16 | 0.1 |
| (2,192) | 1:77:A:LEU:HG | 1:78:A:THR:H | 1 | 0.1 |
| (2,183) | 1:154:A:VAL:HA | 1:157:A:GLN:H | 19 | 0.1 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG21 | 10 | 0.1 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG22 | 10 | 0.1 |
| (2,178) | 1:21:A:ARG:H | 1:23:A:ILE:HG23 | 10 | 0.1 |
| (2,116) | 1:172:A:ARG:H | 1:172:A:ARG:HB3 | 9 | 0.1 |
| (2,101) | 1:151:A:VAL:H | 1:154:A:VAL:H | 2 | 0.1 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD11 | 18 | 0.1 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD12 | 18 | 0.1 |
| (2,78) | 1:142:A:LEU:H | 1:142:A:LEU:HD13 | 18 | 0.1 |
| (2,68) | 1:185:A:GLU:H | 1:186:A:LEU:H | 18 | 0.1 |
| (2,61) | 1:60:A:LEU:HA | 1:117:A:ARG:H | 6 | 0.1 |
| (2,44) | 1:110:A:ARG:H | 1:110:A:ARG:HD3 | 13 | 0.1 |
| (2,15) | 1:96:A:VAL:HB | 1:97:A:PHE:H | 10 | 0.1 |
| (1,99) | 1:96:A:VAL:H | 1:179:A:ARG:O | 12 | 0.1 |
| (1,98) | 1:96:A:VAL:N | 1:179:A:ARG:O | 8 | 0.1 |
| (1,84) | 1:61:A:ILE:H | 1:135:A:LEU:O | 12 | 0.1 |
| (1,84) | 1:61:A:ILE:H | 1:135:A:LEU:O | 17 | 0.1 |

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| Key | Atom-1 | Atom-2 | Model ID | Violation (Å) |
|------------|---------------|---------------|-----------------|----------------------|
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 2 | 0.1 |
| (1,57) | 1:127:A:LEU:O | 1:131:A:TYR:H | 9 | 0.1 |
| (1,47) | 1:105:A:ARG:O | 1:109:A:GLY:H | 20 | 0.1 |
| (1,36) | 1:65:A:TYR:O | 1:69:A:LYS:H | 1 | 0.1 |
| (1,20) | 1:13:A:ALA:O | 1:17:A:LEU:H | 5 | 0.1 |

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

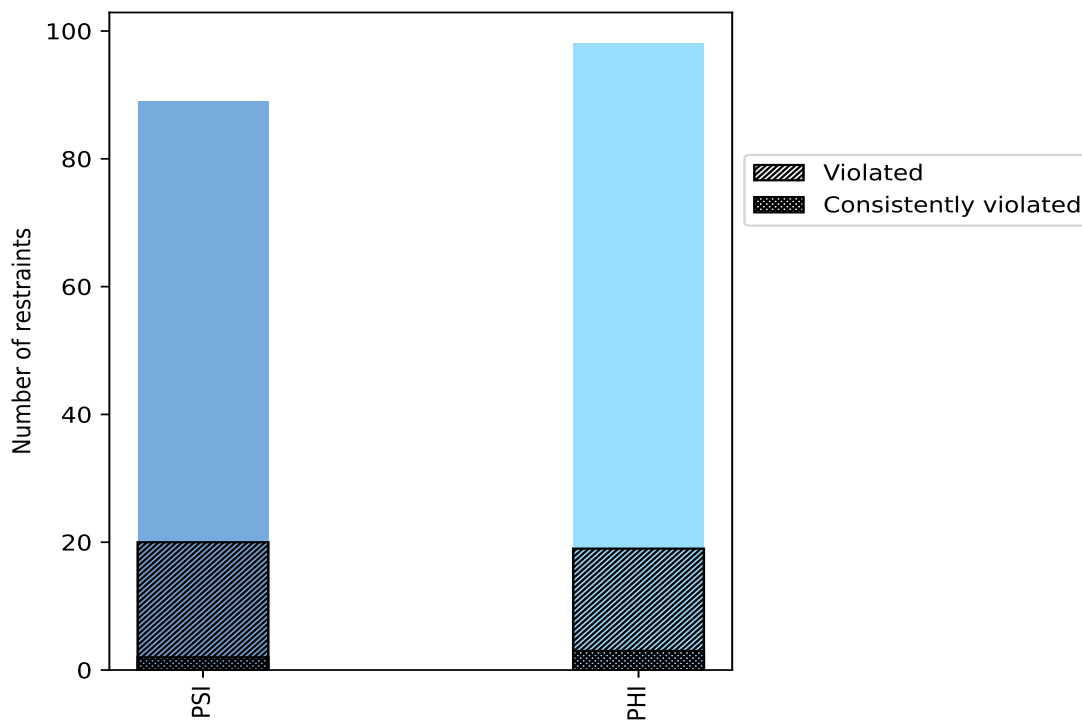
10.1 Summary of dihedral-angle violations [i](#)

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 | 89 | 47.6 | 20 | 22.5 | 10.7 | 2 | 2.2 | 1.1 |
| PHI | 98 | 52.4 | 19 | 19.4 | 10.2 | 3 | 3.1 | 1.6 |
| Total | 187 | 100.0 | 39 | 20.9 | 20.9 | 5 | 2.7 | 2.7 |

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

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



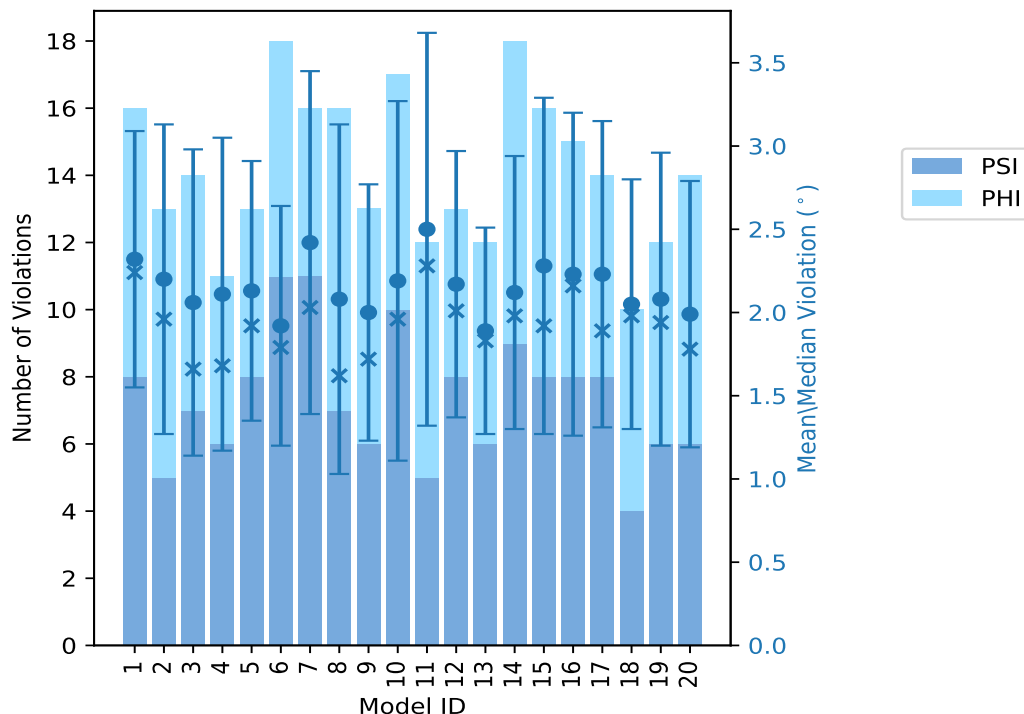
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations | | | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
| | PSI | PHI | Total | | | | |
| 1 | 8 | 8 | 16 | 2.32 | 3.98 | 0.77 | 2.24 |
| 2 | 5 | 8 | 13 | 2.2 | 4.01 | 0.93 | 1.96 |
| 3 | 7 | 7 | 14 | 2.06 | 3.69 | 0.92 | 1.66 |
| 4 | 6 | 5 | 11 | 2.11 | 3.72 | 0.94 | 1.68 |
| 5 | 8 | 5 | 13 | 2.13 | 3.42 | 0.78 | 1.92 |
| 6 | 11 | 7 | 18 | 1.92 | 3.12 | 0.72 | 1.79 |
| 7 | 11 | 5 | 16 | 2.42 | 4.76 | 1.03 | 2.03 |
| 8 | 7 | 9 | 16 | 2.08 | 4.45 | 1.05 | 1.62 |
| 9 | 6 | 7 | 13 | 2.0 | 3.59 | 0.77 | 1.72 |
| 10 | 10 | 7 | 17 | 2.19 | 5.58 | 1.08 | 1.96 |
| 11 | 5 | 7 | 12 | 2.5 | 4.68 | 1.18 | 2.28 |
| 12 | 8 | 5 | 13 | 2.17 | 3.82 | 0.8 | 2.01 |
| 13 | 6 | 6 | 12 | 1.89 | 2.92 | 0.62 | 1.83 |
| 14 | 9 | 9 | 18 | 2.12 | 4.04 | 0.82 | 1.98 |
| 15 | 8 | 8 | 16 | 2.28 | 4.85 | 1.01 | 1.92 |
| 16 | 8 | 7 | 15 | 2.23 | 5.06 | 0.97 | 2.16 |
| 17 | 8 | 6 | 14 | 2.23 | 4.02 | 0.92 | 1.89 |
| 18 | 4 | 6 | 10 | 2.05 | 3.81 | 0.75 | 1.98 |
| 19 | 6 | 6 | 12 | 2.08 | 3.5 | 0.88 | 1.94 |
| 20 | 6 | 8 | 14 | 1.99 | 3.42 | 0.8 | 1.78 |

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



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

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

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

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

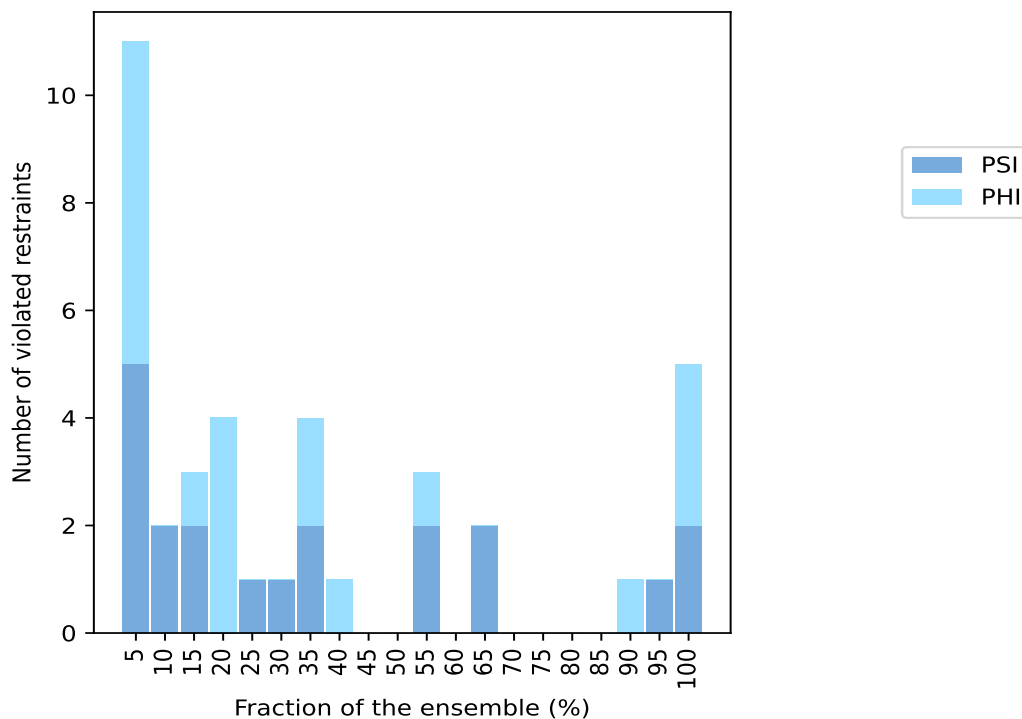
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| Number of violated restraints | | | Fraction of the ensemble | |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI | PHI | Total | Count ¹ | % |
| 0 | 0 | 0 | 12 | 60.0 |
| 2 | 0 | 2 | 13 | 65.0 |
| 0 | 0 | 0 | 14 | 70.0 |
| 0 | 0 | 0 | 15 | 75.0 |
| 0 | 0 | 0 | 16 | 80.0 |
| 0 | 0 | 0 | 17 | 85.0 |
| 0 | 1 | 1 | 18 | 90.0 |
| 1 | 0 | 1 | 19 | 95.0 |
| 2 | 3 | 5 | 20 | 100.0 |

¹ Number of models with violations

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

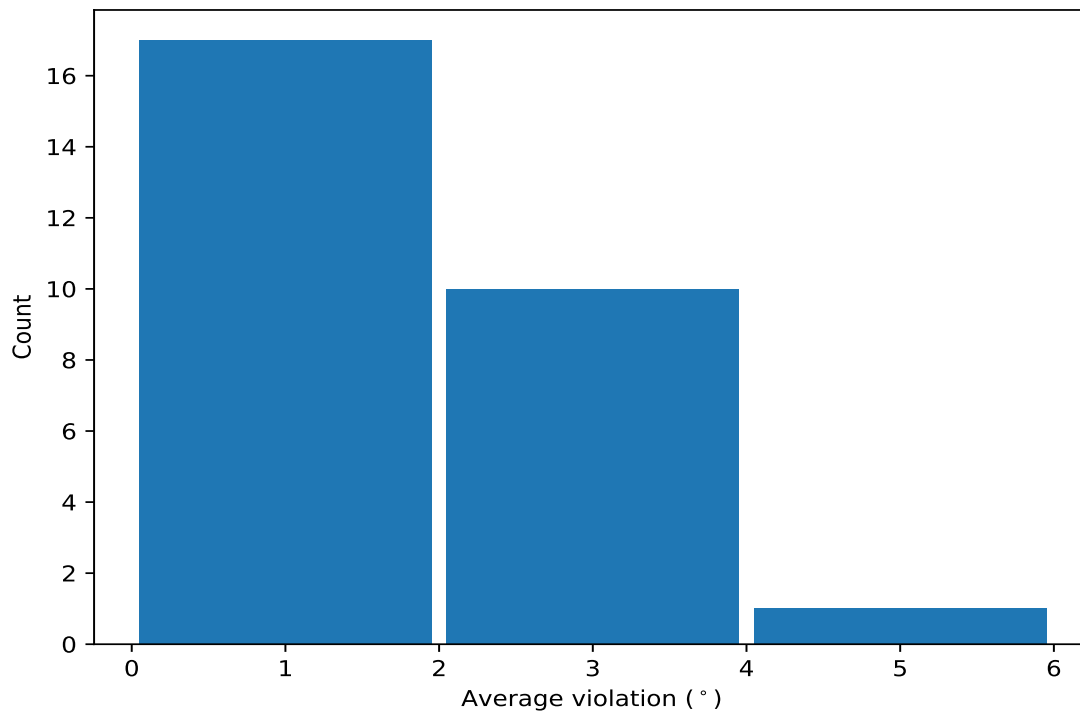


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|------|-----------------|--------|
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 20 | 3.4 | 0.72 | 3.22 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 20 | 3.3 | 0.38 | 3.32 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 20 | 2.3 | 0.52 | 2.4 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 20 | 1.92 | 0.47 | 1.94 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 20 | 1.68 | 0.34 | 1.66 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 19 | 1.49 | 0.26 | 1.41 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 18 | 2.57 | 0.74 | 2.4 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 13 | 1.64 | 0.4 | 1.54 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 13 | 1.33 | 0.21 | 1.31 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 11 | 3.55 | 0.41 | 3.52 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 11 | 2.47 | 1.06 | 2.4 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 11 | 1.63 | 0.42 | 1.71 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 8 | 2.22 | 0.87 | 2.09 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 7 | 3.03 | 0.17 | 2.98 |
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 7 | 1.91 | 0.36 | 1.92 |
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 7 | 1.87 | 0.63 | 2.12 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 7 | 1.29 | 0.22 | 1.22 |
| (1,146) | 1:130:A:ALA:N | 1:130:A:ALA:CA | 1:130:A:ALA:C | 1:131:A:TYR:N | 6 | 1.47 | 0.4 | 1.33 |
| (1,120) | 1:113:A:SER:N | 1:113:A:SER:CA | 1:113:A:SER:C | 1:114:A:LEU:N | 5 | 2.01 | 1.05 | 1.5 |
| (1,173) | 1:159:A:GLY:C | 1:160:A:ALA:N | 1:160:A:ALA:CA | 1:160:A:ALA:C | 4 | 1.46 | 0.29 | 1.46 |

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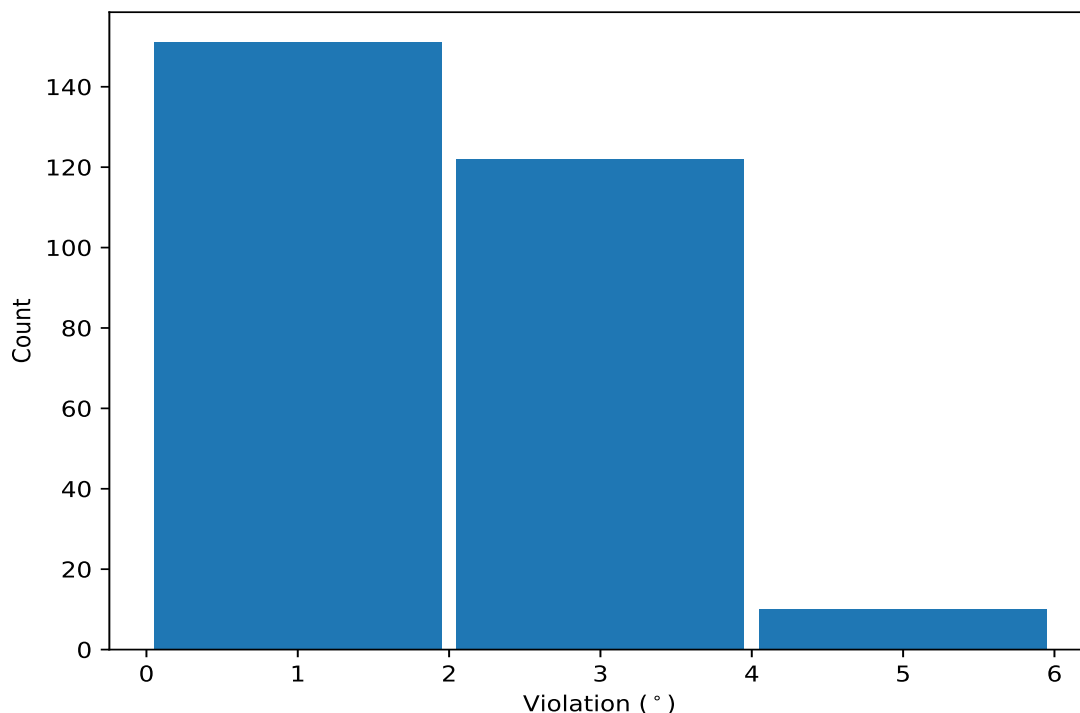
| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Models ¹ | Mean | SD ² | Median |
|---------|---------------|----------------|---------------|---------------|---------------------|------|-----------------|--------|
| (1,105) | 1:92:A:PRO:C | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 4 | 1.34 | 0.34 | 1.2 |
| (1,24) | 1:16:A:VAL:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 4 | 1.26 | 0.11 | 1.27 |
| (1,88) | 1:78:A:THR:C | 1:79:A:ASP:N | 1:79:A:ASP:CA | 1:79:A:ASP:C | 4 | 1.2 | 0.14 | 1.16 |
| (1,104) | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 1:94:A:THR:N | 3 | 2.08 | 0.12 | 2.14 |
| (1,171) | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 1:159:A:GLY:N | 3 | 1.8 | 0.31 | 1.62 |
| (1,27) | 1:20:A:GLU:C | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C | 3 | 1.37 | 0.32 | 1.28 |
| (1,122) | 1:114:A:LEU:N | 1:114:A:LEU:CA | 1:114:A:LEU:C | 1:115:A:ALA:N | 2 | 4.64 | 0.94 | 4.64 |
| (1,19) | 1:15:A:ASP:N | 1:15:A:ASP:CA | 1:15:A:ASP:C | 1:16:A:VAL:N | 2 | 1.18 | 0.02 | 1.18 |

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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,122) | 1:114:A:LEU:N | 1:114:A:LEU:CA | 1:114:A:LEU:C | 1:115:A:ALA:N | 10 | 5.58 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 16 | 5.06 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 15 | 4.85 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 7 | 4.76 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 11 | 4.68 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 8 | 4.45 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 7 | 4.07 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 14 | 4.04 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 17 | 4.02 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 2 | 4.01 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 11 | 3.99 |
| (1,120) | 1:113:A:SER:N | 1:113:A:SER:CA | 1:113:A:SER:C | 1:114:A:LEU:N | 1 | 3.98 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 11 | 3.85 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 15 | 3.83 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 12 | 3.82 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 18 | 3.81 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 17 | 3.78 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 4 | 3.72 |
| (1,122) | 1:114:A:LEU:N | 1:114:A:LEU:CA | 1:114:A:LEU:C | 1:115:A:ALA:N | 7 | 3.71 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 3 | 3.69 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 2 | 3.61 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 2 | 3.61 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 9 | 3.59 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 1 | 3.58 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 16 | 3.52 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 4 | 3.52 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 19 | 3.5 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 14 | 3.49 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 8 | 3.48 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 8 | 3.45 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 19 | 3.44 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 5 | 3.42 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 20 | 3.42 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 17 | 3.42 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 3 | 3.4 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 12 | 3.38 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 7 | 3.37 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 3 | 3.36 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 20 | 3.29 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 11 | 3.28 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 10 | 3.28 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 1 | 3.27 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 8 | 3.22 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 20 | 3.17 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 14 | 3.13 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 8 | 3.13 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 5 | 3.13 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 6 | 3.12 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 6 | 3.08 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 10 | 3.06 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 7 | 3.06 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 15 | 3.05 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 9 | 3.04 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 3 | 3.02 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 4 | 3.01 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 6 | 3.01 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 5 | 2.99 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 9 | 2.98 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 1 | 2.97 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 10 | 2.97 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 19 | 2.95 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 17 | 2.93 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 6 | 2.92 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 13 | 2.92 |
| (1,162) | 1:153:A:GLU:N | 1:153:A:GLU:CA | 1:153:A:GLU:C | 1:154:A:VAL:N | 15 | 2.87 |
| (1,166) | 1:154:A:VAL:C | 1:155:A:ARG:N | 1:155:A:ARG:CA | 1:155:A:ARG:C | 12 | 2.84 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 11 | 2.82 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 12 | 2.82 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 5 | 2.79 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 19 | 2.79 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 4 | 2.78 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 15 | 2.76 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 15 | 2.75 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 13 | 2.71 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 5 | 2.65 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 11 | 2.64 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 14 | 2.64 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 18 | 2.63 |
| (1,107) | 1:93:A:VAL:C | 1:94:A:THR:N | 1:94:A:THR:CA | 1:94:A:THR:C | 14 | 2.61 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 1 | 2.59 |
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 16 | 2.57 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 16 | 2.56 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 3 | 2.56 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 15 | 2.56 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 6 | 2.54 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 10 | 2.54 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 12 | 2.53 |
| (1,178) | 1:178:A:ILE:N | 1:178:A:ILE:CA | 1:178:A:ILE:C | 1:179:A:ARG:N | 1 | 2.5 |
| (1,57) | 1:46:A:LEU:C | 1:47:A:LEU:N | 1:47:A:LEU:CA | 1:47:A:LEU:C | 18 | 2.49 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 7 | 2.48 |
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 5 | 2.47 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 13 | 2.47 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 14 | 2.47 |
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 17 | 2.46 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 13 | 2.42 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 2 | 2.42 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 9 | 2.4 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 6 | 2.4 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 19 | 2.39 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 10 | 2.37 |
| (1,145) | 1:128:A:CYS:C | 1:129:A:GLN:N | 1:129:A:GLN:CA | 1:129:A:GLN:C | 16 | 2.37 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 20 | 2.37 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 9 | 2.34 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 16 | 2.33 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 7 | 2.32 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 20 | 2.31 |
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 1 | 2.25 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 1 | 2.25 |
| (1,171) | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 1:159:A:GLY:N | 10 | 2.24 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1 | 2.24 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 14 | 2.23 |
| (1,146) | 1:130:A:ALA:N | 1:130:A:ALA:CA | 1:130:A:ALA:C | 1:131:A:TYR:N | 10 | 2.22 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 16 | 2.21 |
| (1,104) | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 1:94:A:THR:N | 14 | 2.2 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 2 | 2.17 |
| (1,120) | 1:113:A:SER:N | 1:113:A:SER:CA | 1:113:A:SER:C | 1:114:A:LEU:N | 19 | 2.17 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 4 | 2.17 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 16 | 2.16 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 13 | 2.16 |
| (1,104) | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 1:94:A:THR:N | 17 | 2.14 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 13 | 2.13 |
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 12 | 2.12 |
| (1,82) | 1:66:A:GLU:C | 1:67:A:GLN:N | 1:67:A:GLN:CA | 1:67:A:GLN:C | 18 | 2.12 |
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 7 | 2.09 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 3 | 2.08 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 14 | 2.04 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 2 | 2.04 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 9 | 2.02 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 12 | 2.01 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 18 | 2.01 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 16 | 2.0 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 1 | 2.0 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 16 | 1.97 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 7 | 1.97 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 2 | 1.96 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 10 | 1.96 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 2 | 1.96 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 18 | 1.95 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 7 | 1.95 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 8 | 1.95 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 20 | 1.94 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 1 | 1.93 |
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 15 | 1.92 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 5 | 1.92 |
| (1,105) | 1:92:A:PRO:C | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 14 | 1.92 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 11 | 1.92 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 17 | 1.92 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 15 | 1.91 |
| (1,104) | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 1:94:A:THR:N | 6 | 1.91 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 6 | 1.89 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 2 | 1.87 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 1 | 1.86 |
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 3 | 1.86 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 17 | 1.86 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 20 | 1.83 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 14 | 1.83 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 6 | 1.81 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 16 | 1.8 |
| (1,27) | 1:20:A:GLU:C | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C | 8 | 1.8 |
| (1,173) | 1:159:A:GLY:C | 1:160:A:ALA:N | 1:160:A:ALA:CA | 1:160:A:ALA:C | 8 | 1.79 |
| (1,124) | 1:115:A:ALA:N | 1:115:A:ALA:CA | 1:115:A:ALA:C | 1:116:A:VAL:N | 15 | 1.79 |
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 14 | 1.78 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 11 | 1.77 |
| (1,146) | 1:130:A:ALA:N | 1:130:A:ALA:CA | 1:130:A:ALA:C | 1:131:A:TYR:N | 1 | 1.77 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 6 | 1.77 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 15 | 1.77 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 20 | 1.74 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 7 | 1.73 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 14 | 1.73 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 20 | 1.73 |
| (1,60) | 1:48:A:GLU:C | 1:49:A:LEU:N | 1:49:A:LEU:CA | 1:49:A:LEU:C | 9 | 1.72 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 18 | 1.71 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 10 | 1.71 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 20 | 1.71 |
| (1,173) | 1:159:A:GLY:C | 1:160:A:ALA:N | 1:160:A:ALA:CA | 1:160:A:ALA:C | 17 | 1.7 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 19 | 1.7 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 4 | 1.68 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 15 | 1.67 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 17 | 1.66 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 7 | 1.66 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 7 | 1.65 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 5 | 1.64 |
| (1,171) | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 1:159:A:GLY:N | 5 | 1.62 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 4 | 1.62 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 12 | 1.59 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 17 | 1.58 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 12 | 1.58 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 10 | 1.57 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 2 | 1.57 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 6 | 1.55 |
| (1,171) | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 1:159:A:GLY:N | 9 | 1.54 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 12 | 1.54 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 10 | 1.54 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 13 | 1.53 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 11 | 1.52 |
| (1,17) | 1:14:A:ILE:N | 1:14:A:ILE:CA | 1:14:A:ILE:C | 1:15:A:ASP:N | 7 | 1.51 |
| (1,120) | 1:113:A:SER:N | 1:113:A:SER:CA | 1:113:A:SER:C | 1:114:A:LEU:N | 18 | 1.5 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 17 | 1.5 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 13 | 1.5 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 5 | 1.49 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 12 | 1.47 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 3 | 1.46 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 8 | 1.45 |
| (1,88) | 1:78:A:THR:C | 1:79:A:ASP:N | 1:79:A:ASP:CA | 1:79:A:ASP:C | 1 | 1.43 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 3 | 1.42 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 12 | 1.42 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 1 | 1.41 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 11 | 1.4 |
| (1,80) | 1:65:A:TYR:C | 1:66:A:GLU:N | 1:66:A:GLU:CA | 1:66:A:GLU:C | 14 | 1.4 |
| (1,146) | 1:130:A:ALA:N | 1:130:A:ALA:CA | 1:130:A:ALA:C | 1:131:A:TYR:N | 6 | 1.39 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 3 | 1.39 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 15 | 1.39 |
| (1,24) | 1:16:A:VAL:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 10 | 1.39 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 19 | 1.37 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 10 | 1.37 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 6 | 1.35 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 9 | 1.34 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 16 | 1.34 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 9 | 1.33 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 19 | 1.33 |
| (1,24) | 1:16:A:VAL:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 9 | 1.33 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 8 | 1.32 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 8 | 1.32 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 4 | 1.31 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 9 | 1.31 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 8 | 1.3 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 10 | 1.29 |
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 3 | 1.28 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 2 | 1.28 |
| (1,27) | 1:20:A:GLU:C | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C | 16 | 1.28 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 7 | 1.27 |
| (1,146) | 1:130:A:ALA:N | 1:130:A:ALA:CA | 1:130:A:ALA:C | 1:131:A:TYR:N | 5 | 1.27 |
| (1,105) | 1:92:A:PRO:C | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 8 | 1.26 |
| (1,120) | 1:113:A:SER:N | 1:113:A:SER:CA | 1:113:A:SER:C | 1:114:A:LEU:N | 4 | 1.25 |
| (1,173) | 1:159:A:GLY:C | 1:160:A:ALA:N | 1:160:A:ALA:CA | 1:160:A:ALA:C | 13 | 1.23 |
| (1,88) | 1:78:A:THR:C | 1:79:A:ASP:N | 1:79:A:ASP:CA | 1:79:A:ASP:C | 3 | 1.23 |
| (1,7) | 1:9:A:ALA:N | 1:9:A:ALA:CA | 1:9:A:ALA:C | 1:10:A:ILE:N | 16 | 1.23 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 6 | 1.22 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 13 | 1.22 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 5 | 1.22 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 13 | 1.21 |
| (1,24) | 1:16:A:VAL:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 6 | 1.21 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 14 | 1.2 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 18 | 1.2 |
| (1,19) | 1:15:A:ASP:N | 1:15:A:ASP:CA | 1:15:A:ASP:C | 1:16:A:VAL:N | 6 | 1.2 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 13 | 1.19 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 14 | 1.19 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 15 | 1.18 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 17 | 1.17 |
| (1,164) | 1:153:A:GLU:C | 1:154:A:VAL:N | 1:154:A:VAL:CA | 1:154:A:VAL:C | 20 | 1.17 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 19 | 1.16 |
| (1,19) | 1:15:A:ASP:N | 1:15:A:ASP:CA | 1:15:A:ASP:C | 1:16:A:VAL:N | 7 | 1.16 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 8 | 1.15 |
| (1,121) | 1:112:A:ASP:C | 1:113:A:SER:N | 1:113:A:SER:CA | 1:113:A:SER:C | 1 | 1.15 |
| (1,120) | 1:113:A:SER:N | 1:113:A:SER:CA | 1:113:A:SER:C | 1:114:A:LEU:N | 12 | 1.15 |
| (1,105) | 1:92:A:PRO:C | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 4 | 1.15 |

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| Key | Atom-1 | Atom-2 | Atom-3 | Atom-4 | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 14 | 1.12 |
| (1,173) | 1:159:A:GLY:C | 1:160:A:ALA:N | 1:160:A:ALA:CA | 1:160:A:ALA:C | 9 | 1.11 |
| (1,172) | 1:157:A:GLN:C | 1:158:A:PHE:N | 1:158:A:PHE:CA | 1:158:A:PHE:C | 2 | 1.11 |
| (1,24) | 1:16:A:VAL:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 8 | 1.11 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 18 | 1.1 |
| (1,146) | 1:130:A:ALA:N | 1:130:A:ALA:CA | 1:130:A:ALA:C | 1:131:A:TYR:N | 20 | 1.1 |
| (1,117) | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 1:109:A:GLY:N | 19 | 1.1 |
| (1,182) | 1:180:A:ASP:N | 1:180:A:ASP:CA | 1:180:A:ASP:C | 1:181:A:ALA:N | 6 | 1.09 |
| (1,174) | 1:164:A:VAL:N | 1:164:A:VAL:CA | 1:164:A:VAL:C | 1:165:A:VAL:N | 3 | 1.09 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 15 | 1.09 |
| (1,146) | 1:130:A:ALA:N | 1:130:A:ALA:CA | 1:130:A:ALA:C | 1:131:A:TYR:N | 16 | 1.09 |
| (1,118) | 1:107:A:LEU:C | 1:108:A:THR:N | 1:108:A:THR:CA | 1:108:A:THR:C | 19 | 1.09 |
| (1,88) | 1:78:A:THR:C | 1:79:A:ASP:N | 1:79:A:ASP:CA | 1:79:A:ASP:C | 10 | 1.08 |
| (1,88) | 1:78:A:THR:C | 1:79:A:ASP:N | 1:79:A:ASP:CA | 1:79:A:ASP:C | 15 | 1.08 |
| (1,167) | 1:156:A:ALA:N | 1:156:A:ALA:CA | 1:156:A:ALA:C | 1:157:A:GLN:N | 14 | 1.07 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 8 | 1.07 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 17 | 1.05 |
| (1,77) | 1:65:A:TYR:N | 1:65:A:TYR:CA | 1:65:A:TYR:C | 1:66:A:GLU:N | 4 | 1.05 |
| (1,170) | 1:156:A:ALA:C | 1:157:A:GLN:N | 1:157:A:GLN:CA | 1:157:A:GLN:C | 20 | 1.04 |
| (1,150) | 1:135:A:LEU:N | 1:135:A:LEU:CA | 1:135:A:LEU:C | 1:136:A:VAL:N | 10 | 1.04 |
| (1,105) | 1:92:A:PRO:C | 1:93:A:VAL:N | 1:93:A:VAL:CA | 1:93:A:VAL:C | 11 | 1.04 |
| (1,94) | 1:83:A:GLU:N | 1:83:A:GLU:CA | 1:83:A:GLU:C | 1:84:A:THR:N | 11 | 1.04 |
| (1,27) | 1:20:A:GLU:C | 1:21:A:ARG:N | 1:21:A:ARG:CA | 1:21:A:ARG:C | 20 | 1.04 |
| (1,185) | 1:186:A:LEU:C | 1:187:A:PHE:N | 1:187:A:PHE:CA | 1:187:A:PHE:C | 2 | 1.03 |
| (1,139) | 1:125:A:VAL:C | 1:126:A:ALA:N | 1:126:A:ALA:CA | 1:126:A:ALA:C | 3 | 1.03 |
| (1,96) | 1:84:A:THR:N | 1:84:A:THR:CA | 1:84:A:THR:C | 1:85:A:ILE:N | 5 | 1.03 |
| (1,136) | 1:125:A:VAL:N | 1:125:A:VAL:CA | 1:125:A:VAL:C | 1:126:A:ALA:N | 6 | 1.02 |