



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 04:36 AM UTC

PDB ID : 2MW4 / pdb\_00002mw4  
BMRB ID : 25298  
Title : Tetramerization domain of the Ciona intestinalis p53/p73-b transcription factor protein  
Authors : Heering, J.P.; Jonker, H.R.A.; Loehr, F.; Schwalbe, H.; Doetsch, V.  
Deposited on : 2014-10-27

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

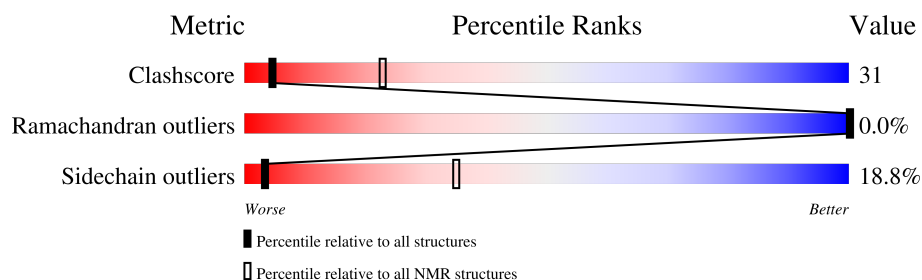
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 22%.

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<br>(#Entries) | NMR archive<br>(#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  $\geq 3$ , 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     | 47     | <div> <div>36%</div> <div>49%</div> <div>11%</div> <div>.</div> </div> |
| 1   | B     | 47     | <div> <div>43%</div> <div>45%</div> <div>13%</div> </div>              |
| 1   | C     | 47     | <div> <div>40%</div> <div>47%</div> <div>13%</div> </div>              |
| 1   | D     | 47     | <div> <div>38%</div> <div>49%</div> <div>13%</div> </div>              |

## 2 Ensemble composition and analysis

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

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

| Well-defined (core) protein residues |                                                                |                   |              |
|--------------------------------------|----------------------------------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                                          | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:105-A:149, B:203-B:249,<br>C:303-C:349, D:403-D:449<br>(186) | 0.41              | 18           |

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3140 atoms, of which 1592 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription factor protein.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 47       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 785   | 243 | 398 | 68 | 74 | 2 |       |
| 1   | B     | 47       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 785   | 243 | 398 | 68 | 74 | 2 |       |
| 1   | C     | 47       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 785   | 243 | 398 | 68 | 74 | 2 |       |
| 1   | D     | 47       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 785   | 243 | 398 | 68 | 74 | 2 |       |

There are 4 discrepancies between the modelled and reference sequences:

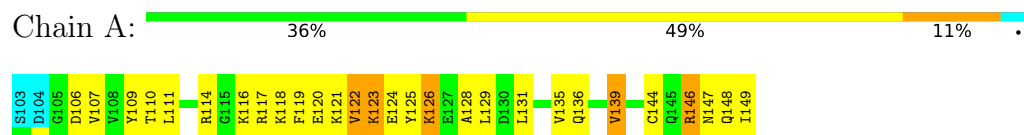
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 103     | SER      | -      | expression tag | UNP Q4H2Z8 |
| B     | 203     | SER      | -      | expression tag | UNP Q4H2Z8 |
| C     | 303     | SER      | -      | expression tag | UNP Q4H2Z8 |
| D     | 403     | SER      | -      | expression tag | UNP Q4H2Z8 |

## 4 Residue-property plots [i](#)

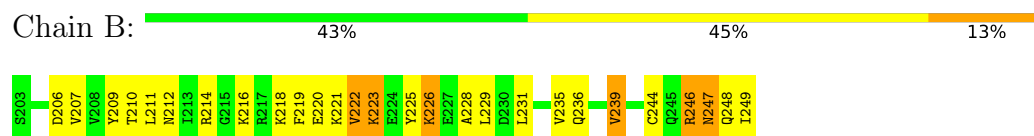
### 4.1 Average score per residue in the NMR ensemble

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.

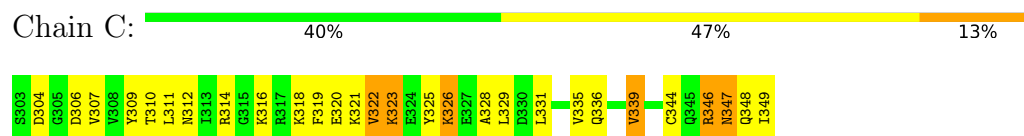
- Molecule 1: Transcription factor protein



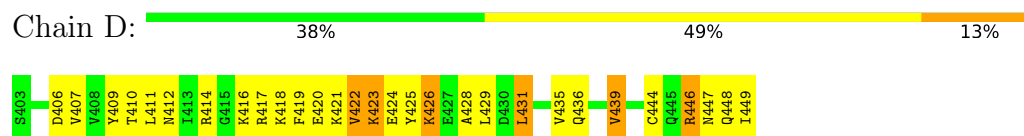
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

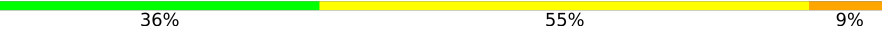
### 4.2.1 Score per residue for model 1

- Molecule 1: Transcription factor protein

Chain A: 



- Molecule 1: Transcription factor protein

Chain B: 

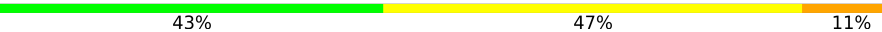


- Molecule 1: Transcription factor protein

Chain C: 



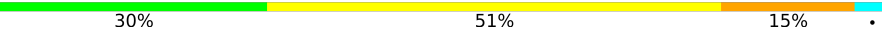
- Molecule 1: Transcription factor protein

Chain D: 



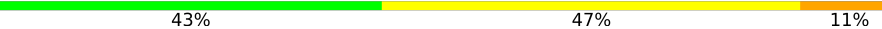
### 4.2.2 Score per residue for model 2

- Molecule 1: Transcription factor protein

Chain A: 



- Molecule 1: Transcription factor protein

Chain B: 



- Molecule 1: Transcription factor protein

Chain C: 



- Molecule 1: Transcription factor protein



#### 4.2.3 Score per residue for model 3

- Molecule 1: Transcription factor protein



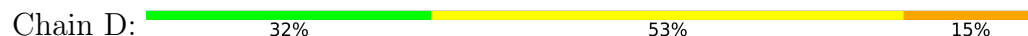
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

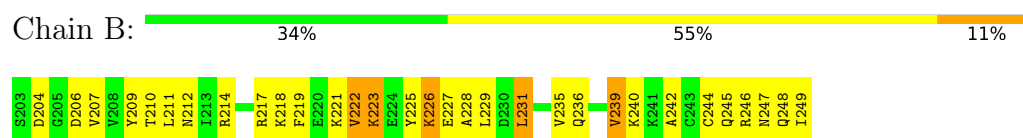


#### 4.2.4 Score per residue for model 4

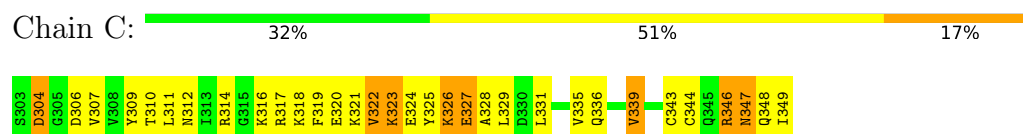
- Molecule 1: Transcription factor protein



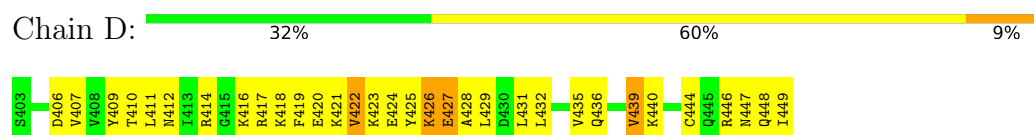
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

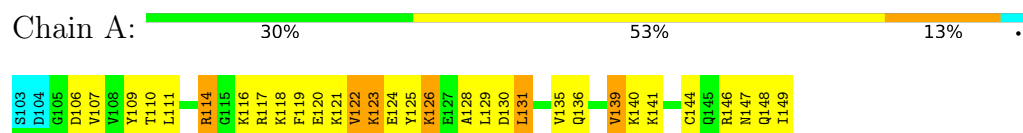


- Molecule 1: Transcription factor protein

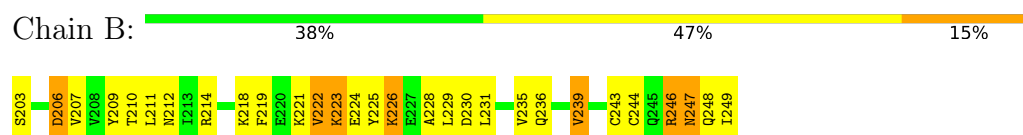


#### 4.2.5 Score per residue for model 5

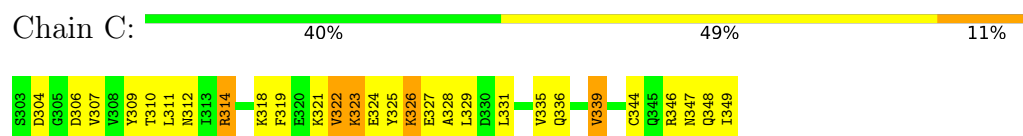
- Molecule 1: Transcription factor protein



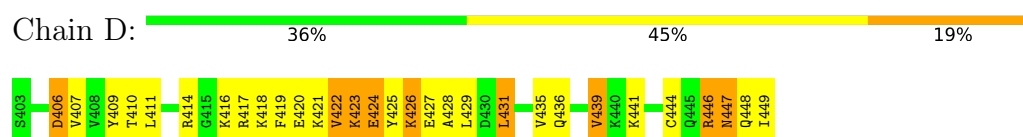
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



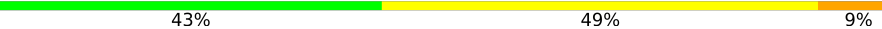
### 4.2.6 Score per residue for model 6

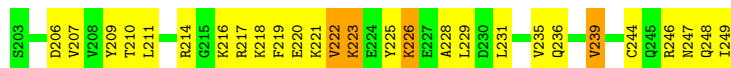
- Molecule 1: Transcription factor protein

Chain A:  36% 51% 9% .



- Molecule 1: Transcription factor protein

Chain B:  43% 49% 9%

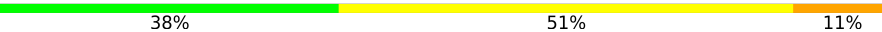


- Molecule 1: Transcription factor protein

Chain C:  47% 43% 11%



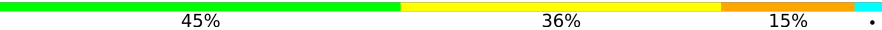
- Molecule 1: Transcription factor protein

Chain D:  38% 51% 11%



### 4.2.7 Score per residue for model 7

- Molecule 1: Transcription factor protein

Chain A:  45% 36% 15% .

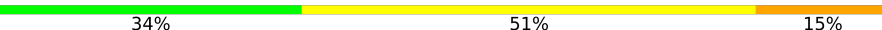


- Molecule 1: Transcription factor protein

Chain B:  40% 53% 6%



- Molecule 1: Transcription factor protein

Chain C:  34% 51% 15%



- Molecule 1: Transcription factor protein

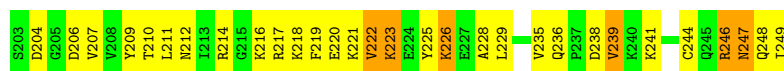


#### 4.2.8 Score per residue for model 8

- Molecule 1: Transcription factor protein



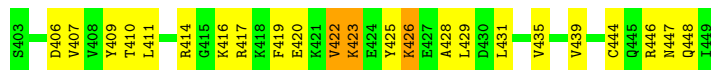
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

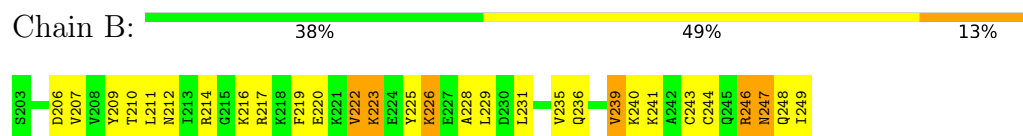


#### 4.2.9 Score per residue for model 9

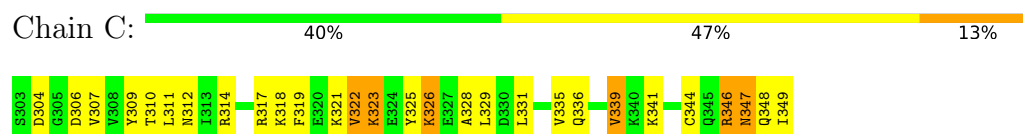
- Molecule 1: Transcription factor protein



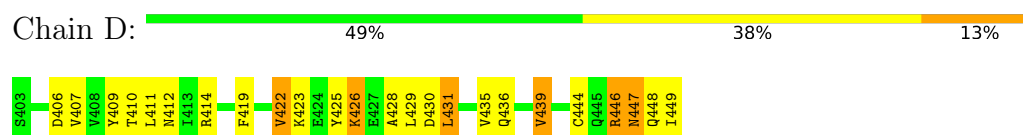
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

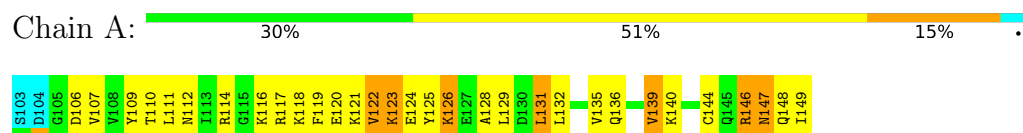


- Molecule 1: Transcription factor protein

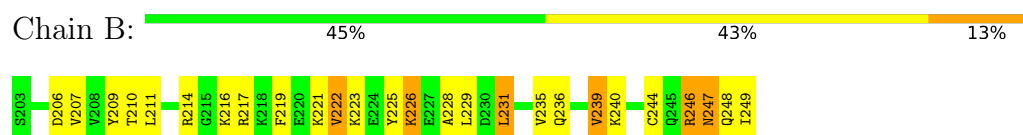


#### 4.2.10 Score per residue for model 10

- Molecule 1: Transcription factor protein



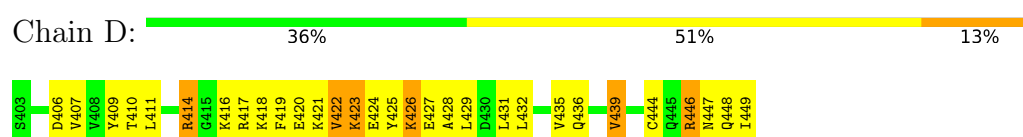
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

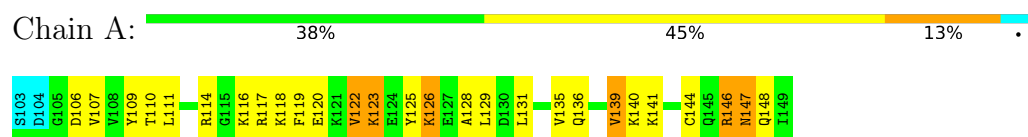


- Molecule 1: Transcription factor protein

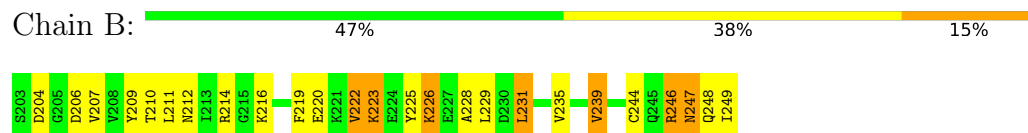


### 4.2.11 Score per residue for model 11

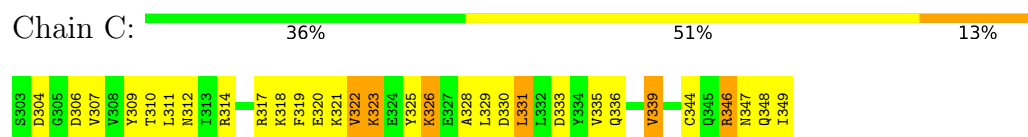
- Molecule 1: Transcription factor protein



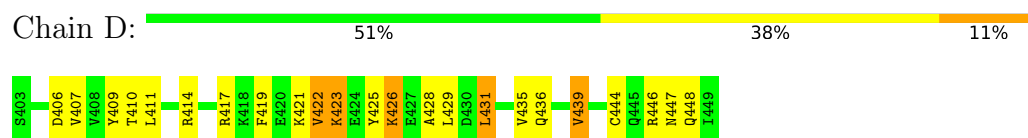
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

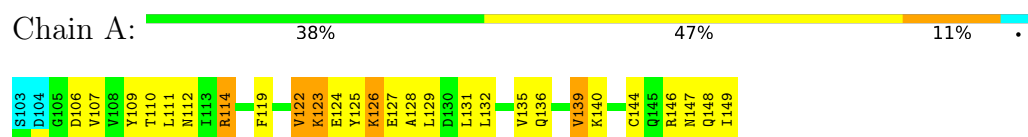


- Molecule 1: Transcription factor protein

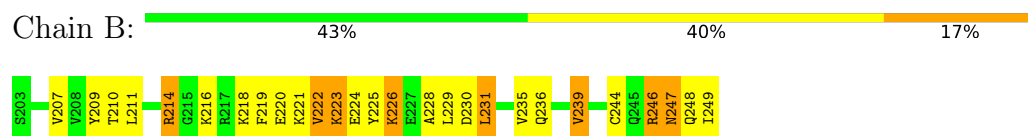


### 4.2.12 Score per residue for model 12

- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein





- Molecule 1: Transcription factor protein



#### 4.2.13 Score per residue for model 13

- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

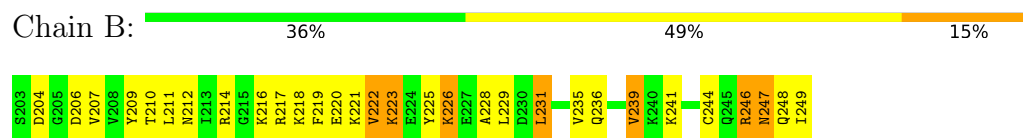


#### 4.2.14 Score per residue for model 14

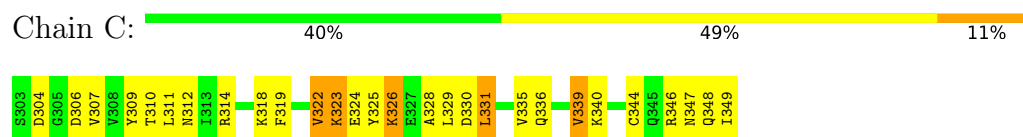
- Molecule 1: Transcription factor protein



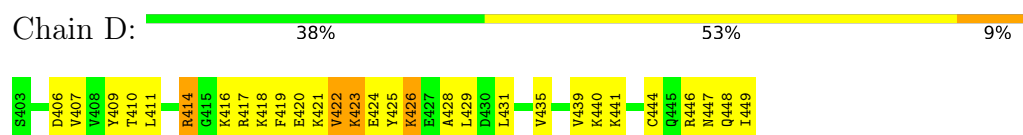
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

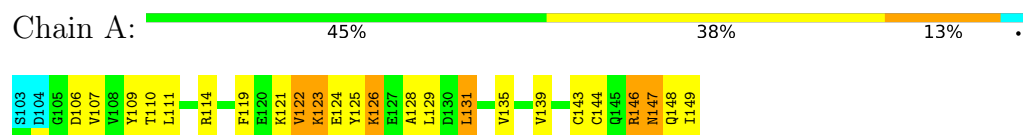


- Molecule 1: Transcription factor protein

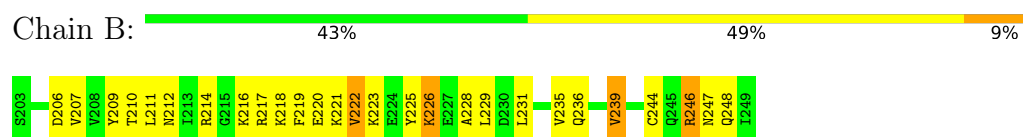


#### 4.2.15 Score per residue for model 15

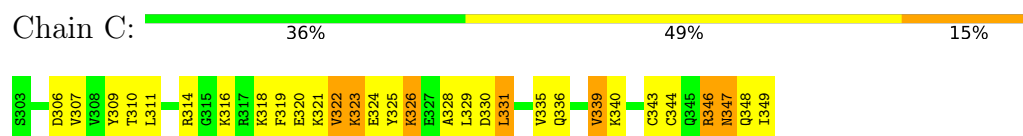
- Molecule 1: Transcription factor protein



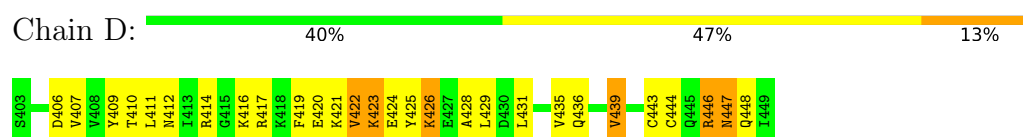
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



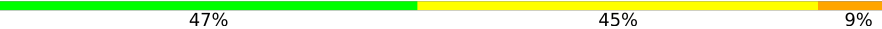
### 4.2.16 Score per residue for model 16

- Molecule 1: Transcription factor protein

Chain A: 



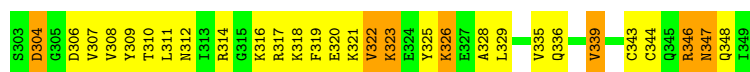
- Molecule 1: Transcription factor protein

Chain B: 

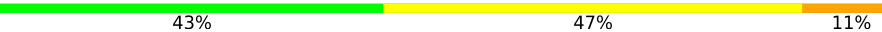


- Molecule 1: Transcription factor protein

Chain C: 



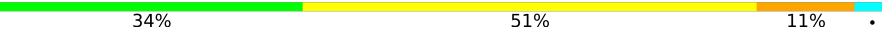
- Molecule 1: Transcription factor protein

Chain D: 



### 4.2.17 Score per residue for model 17

- Molecule 1: Transcription factor protein

Chain A: 



- Molecule 1: Transcription factor protein

Chain B: 



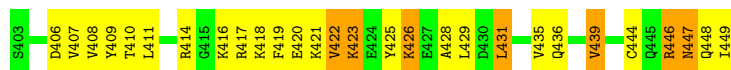
- Molecule 1: Transcription factor protein

Chain C: 



- Molecule 1: Transcription factor protein

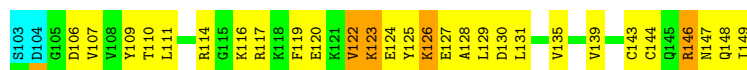
Chain D: 40% 45% 15%



#### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Transcription factor protein

Chain A: 36% 51% 9%



- Molecule 1: Transcription factor protein

Chain B: 45% 45% 11%



- Molecule 1: Transcription factor protein

Chain C: 53% 34% 13%



- Molecule 1: Transcription factor protein

Chain D: 49% 45% 6%



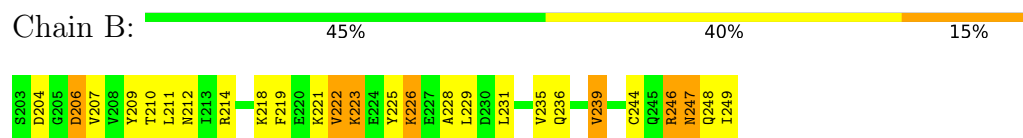
#### 4.2.19 Score per residue for model 19

- Molecule 1: Transcription factor protein

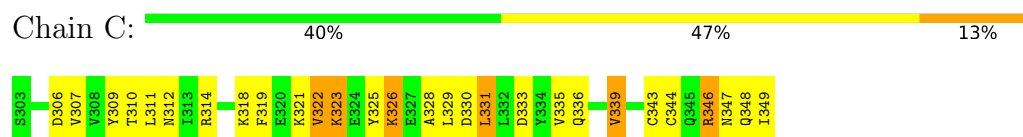
Chain A: 40% 45% 11%



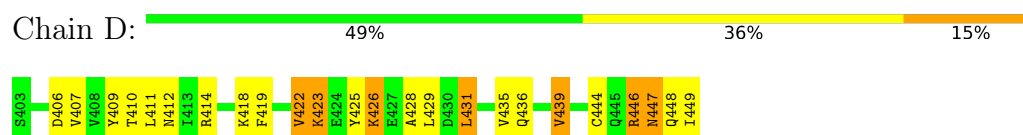
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

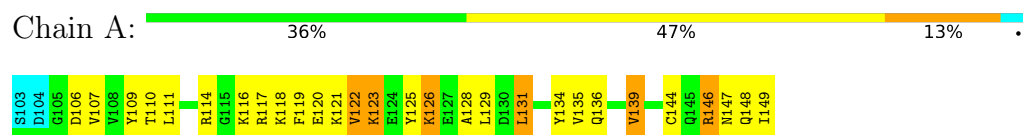


- Molecule 1: Transcription factor protein

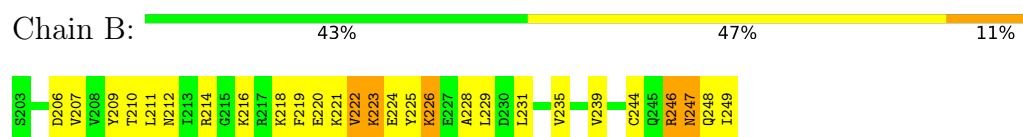


#### 4.2.20 Score per residue for model 20

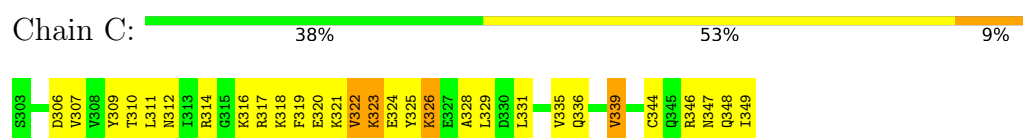
- Molecule 1: Transcription factor protein



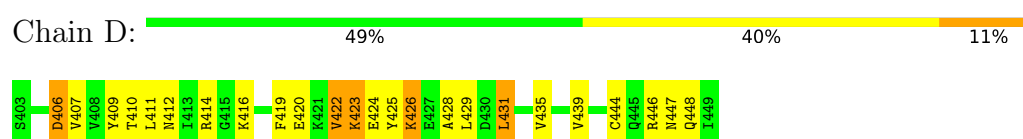
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 3.9     |
| CNS           | structure solution | 1.1     |
| ARIA          | structure solution | 1.2     |
| ARIA          | refinement         | 1.2     |

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                       | 611            |
| Number of shifts mapped to atoms             | 611            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 22%            |

## 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     | 373   | 387      | 387      | 41±4    |
| 1   | B     | 387   | 398      | 395      | 40±4    |
| 1   | C     | 387   | 398      | 395      | 42±4    |
| 1   | D     | 387   | 398      | 395      | 41±5    |
| All | All   | 30680 | 31620    | 31440    | 1905    |

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 31.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:235:VAL:HG11 | 1:D:435:VAL:HG11 | 0.78     | 1.55        | 1      | 20    |
| 1:B:228:ALA:HB1  | 1:D:428:ALA:HB1  | 0.76     | 1.58        | 12     | 20    |
| 1:A:135:VAL:HG11 | 1:C:335:VAL:HG11 | 0.75     | 1.59        | 5      | 20    |
| 1:A:128:ALA:HB1  | 1:C:328:ALA:HB1  | 0.74     | 1.59        | 9      | 20    |
| 1:C:322:VAL:HG12 | 1:D:422:VAL:HG12 | 0.73     | 1.58        | 9      | 20    |
| 1:A:124:GLU:HG2  | 1:D:421:LYS:HD3  | 0.71     | 1.60        | 10     | 10    |
| 1:C:329:LEU:HD12 | 1:D:422:VAL:HG22 | 0.68     | 1.64        | 5      | 19    |
| 1:A:121:LYS:HD3  | 1:D:424:GLU:HG2  | 0.68     | 1.64        | 10     | 7     |
| 1:A:146:ARG:CZ   | 1:A:147:ASN:HB3  | 0.68     | 2.19        | 13     | 13    |
| 1:A:122:VAL:HG12 | 1:B:222:VAL:HG12 | 0.67     | 1.67        | 3      | 20    |
| 1:A:129:LEU:HD12 | 1:B:222:VAL:HG22 | 0.66     | 1.66        | 1      | 20    |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:228:ALA:HB1  | 1:D:428:ALA:CB   | 0.66     | 2.21        | 12     | 20    |
| 1:C:346:ARG:CZ   | 1:C:347:ASN:HB3  | 0.66     | 2.20        | 13     | 11    |
| 1:A:128:ALA:HB1  | 1:C:328:ALA:CB   | 0.65     | 2.21        | 10     | 20    |
| 1:C:310:THR:HG23 | 1:D:410:THR:HG23 | 0.65     | 1.68        | 18     | 20    |
| 1:C:322:VAL:HG22 | 1:D:429:LEU:HD12 | 0.65     | 1.68        | 12     | 19    |
| 1:A:128:ALA:CB   | 1:C:328:ALA:HB1  | 0.64     | 2.23        | 8      | 20    |
| 1:B:228:ALA:CB   | 1:D:428:ALA:HB1  | 0.64     | 2.22        | 6      | 20    |
| 1:A:122:VAL:HG22 | 1:B:229:LEU:HD12 | 0.64     | 1.69        | 11     | 20    |
| 1:D:446:ARG:CZ   | 1:D:447:ASN:HB3  | 0.63     | 2.23        | 13     | 9     |
| 1:D:444:CYS:HA   | 1:D:448:GLN:HB3  | 0.62     | 1.71        | 2      | 20    |
| 1:D:444:CYS:HA   | 1:D:448:GLN:CB   | 0.62     | 2.24        | 2      | 9     |
| 1:A:110:THR:HG23 | 1:B:210:THR:HG23 | 0.62     | 1.72        | 13     | 20    |
| 1:D:423:LYS:O    | 1:D:426:LYS:HG3  | 0.62     | 1.94        | 9      | 19    |
| 1:A:119:PHE:CD2  | 1:B:209:TYR:HB3  | 0.62     | 2.30        | 18     | 13    |
| 1:B:246:ARG:CZ   | 1:B:247:ASN:HB3  | 0.62     | 2.25        | 12     | 12    |
| 1:C:344:CYS:HA   | 1:C:348:GLN:HB3  | 0.61     | 1.72        | 4      | 20    |
| 1:B:223:LYS:O    | 1:B:226:LYS:HG3  | 0.61     | 1.95        | 7      | 20    |
| 1:B:224:GLU:HG2  | 1:C:321:LYS:HD3  | 0.60     | 1.71        | 1      | 6     |
| 1:C:323:LYS:O    | 1:C:326:LYS:HG3  | 0.60     | 1.96        | 9      | 18    |
| 1:B:244:CYS:HA   | 1:B:248:GLN:HB3  | 0.60     | 1.73        | 12     | 20    |
| 1:B:221:LYS:HD3  | 1:C:324:GLU:HG2  | 0.60     | 1.71        | 1      | 7     |
| 1:C:319:PHE:CD2  | 1:D:409:TYR:HB3  | 0.60     | 2.31        | 15     | 8     |
| 1:A:144:CYS:HA   | 1:A:148:GLN:HB3  | 0.59     | 1.74        | 17     | 20    |
| 1:A:109:TYR:HB3  | 1:B:219:PHE:CD2  | 0.59     | 2.33        | 9      | 8     |
| 1:C:319:PHE:CD1  | 1:D:409:TYR:HB3  | 0.59     | 2.33        | 14     | 12    |
| 1:C:309:TYR:HB3  | 1:D:419:PHE:CD2  | 0.58     | 2.33        | 20     | 11    |
| 1:A:119:PHE:CD1  | 1:B:209:TYR:HB3  | 0.58     | 2.33        | 15     | 7     |
| 1:C:314:ARG:HG2  | 1:D:406:ASP:C    | 0.58     | 2.23        | 4      | 19    |
| 1:A:123:LYS:O    | 1:A:126:LYS:HG3  | 0.57     | 2.00        | 10     | 20    |
| 1:D:446:ARG:HD3  | 1:D:447:ASN:OD1  | 0.57     | 1.99        | 3      | 4     |
| 1:A:146:ARG:HD3  | 1:A:147:ASN:OD1  | 0.57     | 1.99        | 9      | 6     |
| 1:A:109:TYR:HB3  | 1:B:219:PHE:CD1  | 0.57     | 2.35        | 17     | 12    |
| 1:A:134:TYR:CD1  | 1:C:346:ARG:HD2  | 0.57     | 2.35        | 20     | 1     |
| 1:A:114:ARG:HG3  | 1:D:449:ILE:HD11 | 0.56     | 1.77        | 4      | 6     |
| 1:B:246:ARG:HD3  | 1:B:247:ASN:OD1  | 0.56     | 2.00        | 15     | 1     |
| 1:C:344:CYS:HA   | 1:C:348:GLN:CB   | 0.56     | 2.30        | 6      | 6     |
| 1:B:234:TYR:CD1  | 1:D:446:ARG:HD2  | 0.56     | 2.36        | 1      | 1     |
| 1:B:244:CYS:HA   | 1:B:248:GLN:CB   | 0.56     | 2.31        | 15     | 7     |
| 1:C:306:ASP:C    | 1:D:414:ARG:HG2  | 0.56     | 2.25        | 2      | 19    |
| 1:A:106:ASP:C    | 1:B:214:ARG:HG2  | 0.55     | 2.25        | 5      | 19    |
| 1:A:116:LYS:HB3  | 1:B:204:ASP:HB3  | 0.55     | 1.78        | 8      | 9     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:135:VAL:CG1  | 1:C:335:VAL:HG11 | 0.55     | 2.30        | 5      | 20    |
| 1:C:346:ARG:HD3  | 1:C:347:ASN:OD1  | 0.55     | 2.02        | 1      | 5     |
| 1:C:309:TYR:HB3  | 1:D:419:PHE:CD1  | 0.54     | 2.37        | 5      | 9     |
| 1:A:114:ARG:HG2  | 1:B:206:ASP:C    | 0.54     | 2.26        | 3      | 16    |
| 1:A:126:LYS:HG2  | 1:B:211:LEU:HD11 | 0.54     | 1.80        | 8      | 20    |
| 1:A:125:TYR:CD1  | 1:C:325:TYR:CD1  | 0.54     | 2.96        | 19     | 20    |
| 1:B:235:VAL:HG11 | 1:D:435:VAL:CG1  | 0.54     | 2.33        | 20     | 20    |
| 1:C:317:ARG:HH11 | 1:C:317:ARG:HG3  | 0.54     | 1.62        | 20     | 1     |
| 1:B:225:TYR:CD1  | 1:D:425:TYR:CD1  | 0.54     | 2.96        | 7      | 20    |
| 1:B:214:ARG:HG3  | 1:C:349:ILE:HD11 | 0.53     | 1.80        | 10     | 6     |
| 1:A:121:LYS:HB3  | 1:B:225:TYR:OH   | 0.53     | 2.03        | 7      | 9     |
| 1:A:111:LEU:HD11 | 1:B:226:LYS:HG2  | 0.53     | 1.81        | 5      | 20    |
| 1:A:135:VAL:HG11 | 1:C:335:VAL:CG1  | 0.53     | 2.33        | 9      | 20    |
| 1:B:243:CYS:SG   | 1:D:431:LEU:HD22 | 0.53     | 2.44        | 5      | 5     |
| 1:C:326:LYS:HG2  | 1:D:411:LEU:HD11 | 0.52     | 1.81        | 16     | 19    |
| 1:D:417:ARG:HD3  | 1:D:420:GLU:OE2  | 0.52     | 2.03        | 8      | 1     |
| 1:C:321:LYS:HD2  | 1:D:429:LEU:HD22 | 0.52     | 1.80        | 7      | 1     |
| 1:B:231:LEU:HD22 | 1:D:443:CYS:SG   | 0.52     | 2.44        | 13     | 6     |
| 1:B:235:VAL:CG1  | 1:D:435:VAL:HG11 | 0.52     | 2.31        | 8      | 20    |
| 1:C:317:ARG:HD3  | 1:C:320:GLU:OE1  | 0.52     | 2.04        | 2      | 4     |
| 1:A:149:ILE:HD11 | 1:D:414:ARG:HG3  | 0.52     | 1.80        | 7      | 7     |
| 1:A:149:ILE:HB   | 1:D:412:ASN:HB2  | 0.52     | 1.82        | 2      | 2     |
| 1:B:236:GLN:O    | 1:B:239:VAL:HG22 | 0.52     | 2.05        | 10     | 13    |
| 1:A:114:ARG:HG2  | 1:B:206:ASP:HA   | 0.51     | 1.82        | 17     | 12    |
| 1:A:144:CYS:HA   | 1:A:148:GLN:CB   | 0.51     | 2.34        | 2      | 9     |
| 1:A:119:PHE:CE1  | 1:B:211:LEU:HD13 | 0.51     | 2.40        | 15     | 4     |
| 1:A:143:CYS:SG   | 1:C:331:LEU:HD22 | 0.51     | 2.46        | 13     | 9     |
| 1:B:216:LYS:O    | 1:B:220:GLU:HG3  | 0.51     | 2.06        | 12     | 11    |
| 1:C:321:LYS:HB3  | 1:D:425:TYR:OH   | 0.50     | 2.06        | 3      | 10    |
| 1:A:136:GLN:O    | 1:A:139:VAL:HG22 | 0.50     | 2.05        | 1      | 13    |
| 1:A:129:LEU:HB3  | 1:B:218:LYS:HG3  | 0.50     | 1.83        | 14     | 11    |
| 1:B:249:ILE:HB   | 1:C:312:ASN:O    | 0.50     | 2.06        | 17     | 17    |
| 1:C:311:LEU:HD11 | 1:D:426:LYS:HG2  | 0.50     | 1.82        | 14     | 20    |
| 1:A:118:LYS:O    | 1:A:122:VAL:HG23 | 0.50     | 2.07        | 2      | 6     |
| 1:A:148:GLN:HG3  | 1:C:330:ASP:OD2  | 0.50     | 2.07        | 15     | 7     |
| 1:C:316:LYS:O    | 1:C:320:GLU:HG3  | 0.50     | 2.06        | 3      | 10    |
| 1:A:131:LEU:HD22 | 1:C:343:CYS:SG   | 0.50     | 2.47        | 18     | 8     |
| 1:A:129:LEU:CD1  | 1:B:222:VAL:HG22 | 0.50     | 2.37        | 15     | 13    |
| 1:A:122:VAL:HG22 | 1:B:229:LEU:CD1  | 0.50     | 2.37        | 7      | 9     |
| 1:A:146:ARG:NE   | 1:A:147:ASN:HB3  | 0.50     | 2.22        | 16     | 4     |
| 1:C:314:ARG:HG2  | 1:D:406:ASP:HA   | 0.50     | 1.84        | 16     | 11    |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:B:235:VAL:HG21 | 1:D:431:LEU:HD12 | 0.50     | 1.83        | 10     | 17    |
| 1:C:306:ASP:HA   | 1:D:414:ARG:HG2  | 0.49     | 1.84        | 19     | 13    |
| 1:B:217:ARG:O    | 1:B:221:LYS:HG3  | 0.49     | 2.08        | 4      | 8     |
| 1:A:148:GLN:HG2  | 1:A:149:ILE:N    | 0.49     | 2.23        | 5      | 2     |
| 1:A:131:LEU:HD12 | 1:C:335:VAL:HG21 | 0.49     | 1.84        | 19     | 16    |
| 1:D:416:LYS:O    | 1:D:420:GLU:HG3  | 0.49     | 2.08        | 14     | 11    |
| 1:A:148:GLN:OE1  | 1:C:327:GLU:HA   | 0.49     | 2.08        | 12     | 1     |
| 1:B:248:GLN:HG3  | 1:D:430:ASP:OD2  | 0.49     | 2.08        | 9      | 5     |
| 1:A:149:ILE:HB   | 1:D:412:ASN:O    | 0.49     | 2.07        | 2      | 11    |
| 1:C:318:LYS:HG3  | 1:D:429:LEU:HB3  | 0.49     | 1.85        | 1      | 13    |
| 1:A:116:LYS:O    | 1:A:120:GLU:HG3  | 0.49     | 2.07        | 1      | 12    |
| 1:B:246:ARG:NE   | 1:B:247:ASN:HB3  | 0.49     | 2.23        | 5      | 6     |
| 1:A:121:LYS:HD3  | 1:B:229:LEU:HD22 | 0.49     | 1.84        | 7      | 1     |
| 1:C:318:LYS:O    | 1:C:322:VAL:HG23 | 0.49     | 2.07        | 9      | 7     |
| 1:A:135:VAL:HG21 | 1:C:331:LEU:HD12 | 0.48     | 1.85        | 19     | 19    |
| 1:C:304:ASP:HB2  | 1:D:417:ARG:HG2  | 0.48     | 1.85        | 14     | 6     |
| 1:A:125:TYR:OH   | 1:B:221:LYS:HB3  | 0.48     | 2.08        | 12     | 12    |
| 1:C:326:LYS:HG2  | 1:D:411:LEU:HD21 | 0.48     | 1.86        | 5      | 17    |
| 1:C:318:LYS:CG   | 1:D:429:LEU:HB3  | 0.48     | 2.38        | 5      | 1     |
| 1:A:148:GLN:HG3  | 1:C:330:ASP:CG   | 0.48     | 2.34        | 11     | 1     |
| 1:B:231:LEU:HD12 | 1:D:435:VAL:HG21 | 0.48     | 1.85        | 3      | 17    |
| 1:D:436:GLN:O    | 1:D:439:VAL:HG22 | 0.48     | 2.08        | 3      | 14    |
| 1:C:336:GLN:O    | 1:C:339:VAL:HG22 | 0.48     | 2.08        | 6      | 15    |
| 1:C:311:LEU:HD13 | 1:D:419:PHE:CE2  | 0.48     | 2.43        | 2      | 9     |
| 1:C:346:ARG:NE   | 1:C:347:ASN:HB3  | 0.48     | 2.24        | 12     | 5     |
| 1:B:230:ASP:OD2  | 1:D:448:GLN:HG3  | 0.48     | 2.09        | 18     | 3     |
| 1:B:217:ARG:HD3  | 1:B:220:GLU:OE1  | 0.48     | 2.08        | 6      | 1     |
| 1:A:119:PHE:O    | 1:A:123:LYS:HB3  | 0.48     | 2.09        | 3      | 6     |
| 1:D:418:LYS:O    | 1:D:422:VAL:HG23 | 0.48     | 2.09        | 10     | 8     |
| 1:A:106:ASP:HA   | 1:B:214:ARG:HG2  | 0.47     | 1.85        | 20     | 9     |
| 1:A:117:ARG:O    | 1:A:121:LYS:HG3  | 0.47     | 2.09        | 10     | 2     |
| 1:B:247:ASN:C    | 1:B:247:ASN:HD22 | 0.47     | 2.16        | 18     | 1     |
| 1:B:249:ILE:HD11 | 1:C:314:ARG:HG3  | 0.47     | 1.87        | 3      | 5     |
| 1:C:325:TYR:OH   | 1:D:421:LYS:HB3  | 0.47     | 2.10        | 3      | 11    |
| 1:A:126:LYS:HG2  | 1:B:211:LEU:HD21 | 0.47     | 1.86        | 14     | 18    |
| 1:C:341:LYS:O    | 1:C:344:CYS:HB3  | 0.47     | 2.10        | 2      | 4     |
| 1:B:212:ASN:O    | 1:C:349:ILE:HB   | 0.47     | 2.09        | 20     | 12    |
| 1:A:116:LYS:HB3  | 1:B:204:ASP:CB   | 0.47     | 2.40        | 19     | 3     |
| 1:A:111:LEU:HD13 | 1:B:219:PHE:CE2  | 0.46     | 2.45        | 3      | 7     |
| 1:C:317:ARG:O    | 1:C:321:LYS:HG3  | 0.46     | 2.10        | 7      | 5     |
| 1:C:322:VAL:HG11 | 1:D:426:LYS:HB3  | 0.46     | 1.86        | 5      | 2     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:D:417:ARG:O    | 1:D:421:LYS:HG3  | 0.46     | 2.11        | 12     | 12    |
| 1:C:311:LEU:HD13 | 1:D:419:PHE:CE1  | 0.46     | 2.45        | 5      | 5     |
| 1:C:340:LYS:NZ   | 1:C:340:LYS:HB3  | 0.46     | 2.25        | 10     | 3     |
| 1:C:329:LEU:CD1  | 1:D:422:VAL:HG22 | 0.46     | 2.39        | 20     | 13    |
| 1:A:110:THR:HG23 | 1:B:210:THR:CG2  | 0.46     | 2.41        | 11     | 10    |
| 1:A:112:ASN:HB2  | 1:D:449:ILE:HB   | 0.46     | 1.88        | 2      | 1     |
| 1:C:304:ASP:HB2  | 1:D:416:LYS:HB3  | 0.46     | 1.88        | 16     | 1     |
| 1:C:304:ASP:HB3  | 1:D:416:LYS:HB3  | 0.46     | 1.87        | 2      | 7     |
| 1:C:319:PHE:CE2  | 1:D:411:LEU:HD13 | 0.46     | 2.46        | 7      | 8     |
| 1:A:118:LYS:HG3  | 1:B:229:LEU:HB3  | 0.46     | 1.86        | 3      | 9     |
| 1:A:117:ARG:HD3  | 1:A:120:GLU:OE1  | 0.46     | 2.11        | 10     | 7     |
| 1:A:128:ALA:HB1  | 1:C:328:ALA:C    | 0.46     | 2.35        | 15     | 14    |
| 1:C:329:LEU:HB3  | 1:D:418:LYS:HG3  | 0.46     | 1.87        | 3      | 13    |
| 1:A:117:ARG:HA   | 1:A:120:GLU:OE1  | 0.46     | 2.10        | 17     | 1     |
| 1:A:110:THR:CG2  | 1:B:210:THR:HG23 | 0.46     | 2.40        | 8      | 16    |
| 1:A:119:PHE:CE2  | 1:B:211:LEU:HD13 | 0.46     | 2.46        | 7      | 13    |
| 1:C:319:PHE:O    | 1:C:323:LYS:HB3  | 0.46     | 2.11        | 3      | 9     |
| 1:D:441:LYS:O    | 1:D:444:CYS:HB3  | 0.46     | 2.11        | 14     | 2     |
| 1:C:304:ASP:CB   | 1:D:416:LYS:HB3  | 0.46     | 2.41        | 2      | 1     |
| 1:A:140:LYS:HB3  | 1:A:140:LYS:NZ   | 0.45     | 2.27        | 2      | 4     |
| 1:A:112:ASN:O    | 1:D:449:ILE:HB   | 0.45     | 2.12        | 17     | 6     |
| 1:C:316:LYS:HB3  | 1:D:404:ASP:HB3  | 0.45     | 1.89        | 2      | 4     |
| 1:B:228:ALA:HB1  | 1:D:428:ALA:C    | 0.45     | 2.36        | 15     | 10    |
| 1:C:347:ASN:C    | 1:C:347:ASN:HD22 | 0.45     | 2.18        | 8      | 3     |
| 1:A:128:ALA:C    | 1:C:328:ALA:HB1  | 0.45     | 2.36        | 11     | 14    |
| 1:C:310:THR:HG23 | 1:D:410:THR:CG2  | 0.45     | 2.40        | 18     | 14    |
| 1:A:111:LEU:HD21 | 1:B:226:LYS:HG2  | 0.45     | 1.89        | 5      | 14    |
| 1:B:218:LYS:O    | 1:B:222:VAL:HG23 | 0.45     | 2.12        | 12     | 9     |
| 1:B:240:LYS:NZ   | 1:B:240:LYS:HB3  | 0.45     | 2.27        | 10     | 3     |
| 1:B:231:LEU:O    | 1:B:235:VAL:HG22 | 0.45     | 2.12        | 3      | 2     |
| 1:B:228:ALA:C    | 1:D:428:ALA:HB1  | 0.45     | 2.37        | 3      | 10    |
| 1:C:311:LEU:HD21 | 1:D:426:LYS:HG2  | 0.45     | 1.89        | 5      | 19    |
| 1:A:111:LEU:HD13 | 1:B:219:PHE:CE1  | 0.44     | 2.48        | 19     | 3     |
| 1:C:346:ARG:NH1  | 1:C:347:ASN:HB3  | 0.44     | 2.26        | 11     | 1     |
| 1:A:130:ASP:OD2  | 1:C:348:GLN:HG3  | 0.44     | 2.13        | 18     | 3     |
| 1:D:436:GLN:HB2  | 1:D:439:VAL:HG13 | 0.44     | 1.89        | 4      | 2     |
| 1:B:249:ILE:HB   | 1:C:312:ASN:HB2  | 0.44     | 1.88        | 5      | 3     |
| 1:B:230:ASP:CG   | 1:D:448:GLN:HG3  | 0.44     | 2.37        | 12     | 2     |
| 1:C:304:ASP:CB   | 1:D:417:ARG:HG2  | 0.44     | 2.42        | 12     | 2     |
| 1:D:441:LYS:O    | 1:D:444:CYS:HB2  | 0.44     | 2.13        | 3      | 2     |
| 1:A:129:LEU:HD22 | 1:B:221:LYS:HD2  | 0.44     | 1.90        | 19     | 1     |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:D:446:ARG:NE   | 1:D:447:ASN:HB3  | 0.44     | 2.28        | 5      | 1     |
| 1:C:322:VAL:HG22 | 1:D:429:LEU:CD1  | 0.44     | 2.43        | 7      | 10    |
| 1:A:123:LYS:HD3  | 1:A:124:GLU:N    | 0.44     | 2.27        | 12     | 2     |
| 1:C:319:PHE:CE1  | 1:D:411:LEU:HD13 | 0.43     | 2.48        | 8      | 8     |
| 1:C:310:THR:CG2  | 1:D:410:THR:HG23 | 0.43     | 2.43        | 5      | 5     |
| 1:A:149:ILE:HD11 | 1:D:414:ARG:HB2  | 0.43     | 1.90        | 4      | 1     |
| 1:C:335:VAL:HB   | 1:C:339:VAL:HG21 | 0.43     | 1.90        | 12     | 1     |
| 1:B:239:VAL:HG23 | 1:D:431:LEU:HD11 | 0.43     | 1.90        | 7      | 5     |
| 1:A:141:LYS:O    | 1:A:144:CYS:HB2  | 0.43     | 2.12        | 5      | 1     |
| 1:C:331:LEU:O    | 1:C:335:VAL:HG22 | 0.43     | 2.13        | 20     | 1     |
| 1:C:336:GLN:HB2  | 1:C:339:VAL:HG13 | 0.43     | 1.90        | 16     | 4     |
| 1:A:132:LEU:HD22 | 1:A:140:LYS:HE2  | 0.43     | 1.90        | 12     | 1     |
| 1:B:241:LYS:O    | 1:B:244:CYS:HB3  | 0.43     | 2.13        | 8      | 5     |
| 1:D:419:PHE:O    | 1:D:423:LYS:HB3  | 0.43     | 2.14        | 5      | 3     |
| 1:A:122:VAL:HG11 | 1:B:226:LYS:HB3  | 0.43     | 1.90        | 4      | 2     |
| 1:B:212:ASN:HB2  | 1:C:349:ILE:HB   | 0.42     | 1.90        | 14     | 1     |
| 1:C:314:ARG:HG2  | 1:D:406:ASP:CA   | 0.42     | 2.44        | 4      | 6     |
| 1:C:326:LYS:HB3  | 1:D:422:VAL:HG11 | 0.42     | 1.90        | 9      | 1     |
| 1:A:126:LYS:HB3  | 1:B:222:VAL:HG11 | 0.42     | 1.91        | 2      | 1     |
| 1:D:432:LEU:HD22 | 1:D:440:LYS:HE2  | 0.42     | 1.91        | 4      | 1     |
| 1:B:231:LEU:HD11 | 1:D:439:VAL:HG23 | 0.42     | 1.91        | 19     | 3     |
| 1:A:136:GLN:HB2  | 1:A:139:VAL:HG13 | 0.42     | 1.92        | 16     | 4     |
| 1:A:131:LEU:HD11 | 1:C:339:VAL:HG23 | 0.42     | 1.90        | 7      | 2     |
| 1:A:114:ARG:HG2  | 1:B:206:ASP:CA   | 0.42     | 2.44        | 17     | 3     |
| 1:B:231:LEU:HD21 | 1:D:440:LYS:HA   | 0.42     | 1.91        | 12     | 1     |
| 1:B:242:ALA:HA   | 1:B:245:GLN:HG2  | 0.42     | 1.90        | 4      | 1     |
| 1:A:139:VAL:HG23 | 1:C:331:LEU:HD11 | 0.42     | 1.91        | 11     | 1     |
| 1:A:117:ARG:HG2  | 1:B:204:ASP:HB2  | 0.42     | 1.90        | 4      | 2     |
| 1:C:348:GLN:HG2  | 1:C:349:ILE:N    | 0.42     | 2.29        | 10     | 1     |
| 1:A:132:LEU:HG   | 1:C:328:ALA:HA   | 0.42     | 1.92        | 10     | 3     |
| 1:D:448:GLN:HG2  | 1:D:449:ILE:N    | 0.41     | 2.30        | 19     | 1     |
| 1:D:426:LYS:HE2  | 1:D:426:LYS:HB2  | 0.41     | 1.77        | 8      | 2     |
| 1:B:228:ALA:HA   | 1:D:432:LEU:HG   | 0.41     | 1.91        | 10     | 4     |
| 1:D:431:LEU:O    | 1:D:435:VAL:HG22 | 0.41     | 2.15        | 7      | 1     |
| 1:A:140:LYS:HG2  | 1:C:331:LEU:HD21 | 0.41     | 1.91        | 11     | 1     |
| 1:A:141:LYS:O    | 1:A:144:CYS:HB3  | 0.41     | 2.14        | 11     | 2     |
| 1:A:139:VAL:CG2  | 1:C:331:LEU:HD11 | 0.41     | 2.45        | 11     | 1     |
| 1:C:306:ASP:CA   | 1:D:414:ARG:HG2  | 0.41     | 2.46        | 19     | 1     |
| 1:A:147:ASN:HD22 | 1:A:147:ASN:N    | 0.41     | 2.14        | 2      | 1     |
| 1:A:118:LYS:HA   | 1:A:121:LYS:HD2  | 0.41     | 1.92        | 7      | 1     |
| 1:A:132:LEU:HD23 | 1:C:331:LEU:HG   | 0.41     | 1.93        | 13     | 1     |

*Continued on next page...*

Continued from previous page...

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:106:ASP:CA   | 1:B:214:ARG:HG2  | 0.41     | 2.45        | 1      | 2     |
| 1:C:346:ARG:HE   | 1:C:346:ARG:C    | 0.41     | 2.23        | 8      | 1     |
| 1:A:135:VAL:CG2  | 1:C:331:LEU:HD12 | 0.41     | 2.46        | 5      | 1     |
| 1:A:117:ARG:HD3  | 1:A:120:GLU:OE2  | 0.41     | 2.15        | 11     | 1     |
| 1:B:236:GLN:HB2  | 1:B:239:VAL:HG13 | 0.41     | 1.93        | 12     | 2     |
| 1:C:329:LEU:HD22 | 1:D:421:LYS:HD2  | 0.41     | 1.92        | 14     | 1     |
| 1:A:149:ILE:HD11 | 1:C:308:VAL:HG22 | 0.41     | 1.92        | 16     | 1     |
| 1:C:323:LYS:HD3  | 1:C:324:GLU:N    | 0.40     | 2.31        | 3      | 1     |
| 1:A:140:LYS:NZ   | 1:C:327:GLU:OE1  | 0.40     | 2.55        | 4      | 1     |
| 1:B:248:GLN:NE2  | 1:D:427:GLU:HA   | 0.40     | 2.31        | 6      | 1     |
| 1:C:313:ILE:HD13 | 1:C:322:VAL:CG2  | 0.40     | 2.47        | 13     | 1     |
| 1:A:131:LEU:O    | 1:A:135:VAL:HG22 | 0.40     | 2.15        | 7      | 1     |
| 1:C:314:ARG:HG3  | 1:D:408:VAL:HG22 | 0.40     | 1.92        | 17     | 1     |
| 1:B:240:LYS:NZ   | 1:D:427:GLU:OE1  | 0.40     | 2.54        | 4      | 1     |
| 1:B:248:GLN:HG3  | 1:D:430:ASP:CG   | 0.40     | 2.42        | 7      | 1     |
| 1:B:217:ARG:HD3  | 1:B:220:GLU:OE2  | 0.40     | 2.16        | 9      | 1     |
| 1:D:417:ARG:HD3  | 1:D:420:GLU:OE1  | 0.40     | 2.15        | 15     | 2     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured     | Allowed    | Outliers   | Percentiles |     |
|-----|-------|-----------------|--------------|------------|------------|-------------|-----|
| 1   | A     | 44/47 (94%)     | 41±1 (93±1%) | 3±1 (7±1%) | 0±0 (0±0%) | 100         | 100 |
| 1   | B     | 45/47 (96%)     | 41±1 (91±2%) | 4±1 (9±2%) | 0±0 (0±0%) | 49          | 83  |
| 1   | C     | 45/47 (96%)     | 41±0 (91±1%) | 4±0 (9±1%) | 0±0 (0±0%) | 100         | 100 |
| 1   | D     | 45/47 (96%)     | 41±1 (91±2%) | 4±1 (9±2%) | 0±0 (0±0%) | 100         | 100 |
| All | All   | 3580/3760 (95%) | 3271 (91%)   | 308 (9%)   | 1 (0%)     | 100         | 100 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 208 | VAL  | 1              |

### 6.3.2 Protein sidechains ⓘ

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

| Mol | Chain | Analysed        | Rotameric    | Outliers    | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|-------------|----|
| 1   | A     | 41/43 (95%)     | 33±1 (81±2%) | 8±1 (19±2%) | 3           | 34 |
| 1   | B     | 43/43 (100%)    | 35±1 (82±2%) | 8±1 (18±2%) | 4           | 36 |
| 1   | C     | 43/43 (100%)    | 35±1 (81±3%) | 8±1 (19±3%) | 3           | 34 |
| 1   | D     | 43/43 (100%)    | 35±1 (81±3%) | 8±1 (19±3%) | 3           | 35 |
| All | All   | 3400/3440 (99%) | 2762 (81%)   | 638 (19%)   | 3           | 35 |

All 62 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     | 107 | VAL  | 20             |
| 1   | A     | 122 | VAL  | 20             |
| 1   | A     | 123 | LYS  | 20             |
| 1   | A     | 126 | LYS  | 20             |
| 1   | A     | 139 | VAL  | 20             |
| 1   | A     | 146 | ARG  | 20             |
| 1   | B     | 207 | VAL  | 20             |
| 1   | B     | 222 | VAL  | 20             |
| 1   | B     | 226 | LYS  | 20             |
| 1   | B     | 246 | ARG  | 20             |
| 1   | C     | 307 | VAL  | 20             |
| 1   | C     | 322 | VAL  | 20             |
| 1   | C     | 323 | LYS  | 20             |
| 1   | C     | 326 | LYS  | 20             |
| 1   | C     | 339 | VAL  | 20             |
| 1   | D     | 407 | VAL  | 20             |
| 1   | D     | 422 | VAL  | 20             |
| 1   | D     | 426 | LYS  | 20             |
| 1   | D     | 439 | VAL  | 20             |
| 1   | B     | 239 | VAL  | 19             |
| 1   | C     | 346 | ARG  | 19             |
| 1   | D     | 446 | ARG  | 19             |
| 1   | B     | 247 | ASN  | 18             |
| 1   | D     | 423 | LYS  | 18             |
| 1   | B     | 223 | LYS  | 16             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | C     | 347 | ASN  | 14             |
| 1   | D     | 447 | ASN  | 14             |
| 1   | A     | 147 | ASN  | 13             |
| 1   | D     | 431 | LEU  | 11             |
| 1   | C     | 331 | LEU  | 10             |
| 1   | A     | 131 | LEU  | 9              |
| 1   | B     | 231 | LEU  | 8              |
| 1   | C     | 327 | GLU  | 6              |
| 1   | A     | 114 | ARG  | 6              |
| 1   | D     | 427 | GLU  | 5              |
| 1   | A     | 127 | GLU  | 5              |
| 1   | D     | 414 | ARG  | 4              |
| 1   | C     | 304 | ASP  | 4              |
| 1   | D     | 424 | GLU  | 4              |
| 1   | B     | 227 | GLU  | 3              |
| 1   | C     | 324 | GLU  | 3              |
| 1   | B     | 206 | ASP  | 3              |
| 1   | B     | 214 | ARG  | 2              |
| 1   | C     | 306 | ASP  | 2              |
| 1   | B     | 240 | LYS  | 2              |
| 1   | C     | 314 | ARG  | 2              |
| 1   | D     | 406 | ASP  | 2              |
| 1   | A     | 140 | LYS  | 2              |
| 1   | C     | 333 | ASP  | 2              |
| 1   | A     | 149 | ILE  | 1              |
| 1   | B     | 224 | GLU  | 1              |
| 1   | D     | 449 | ILE  | 1              |
| 1   | C     | 348 | GLN  | 1              |
| 1   | B     | 203 | SER  | 1              |
| 1   | A     | 124 | GLU  | 1              |
| 1   | A     | 121 | LYS  | 1              |
| 1   | B     | 238 | ASP  | 1              |
| 1   | A     | 106 | ASP  | 1              |
| 1   | D     | 448 | GLN  | 1              |
| 1   | D     | 440 | LYS  | 1              |
| 1   | C     | 340 | LYS  | 1              |
| 1   | B     | 249 | ILE  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 23% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

|                                         |     |
|-----------------------------------------|-----|
| Total number of shifts                  | 611 |
| Number of shifts mapped to atoms        | 611 |
| Number of unparsed shifts               | 0   |
| Number of shifts with mapping errors    | 0   |
| Number of shifts with mapping warnings  | 0   |
| Number of shift outliers (ShiftChecker) | 0   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 47       | $-0.61 \pm 0.17$                | Should be checked          |
| $^{13}\text{C}_\beta$  | 45       | $0.02 \pm 0.18$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 45       | $-0.06 \pm 0.11$                | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 45       | $-0.65 \pm 0.37$                | None needed (imprecise)    |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 22%, i.e. 597 atoms were assigned a chemical shift out of a possible 2679. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 223/930 (24%)  | 91/376 (24%)   | 88/372 (24%)    | 44/182 (24%)    |
| Sidechain | 340/1601 (21%) | 232/1020 (23%) | 107/497 (22%)   | 1/84 (1%)       |

*Continued on next page...*

Continued from previous page...

|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 34/148 (23%)   | 17/68 (25%)    | 17/80 (21%)     | 0/0 (—%)        |
| Overall  | 597/2679 (22%) | 340/1464 (23%) | 212/949 (22%)   | 45/266 (17%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 23%, i.e. 611 atoms were assigned a chemical shift out of a possible 2696. 0 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 231/940 (25%)  | 94/380 (25%)   | 92/376 (24%)    | 45/184 (24%)    |
| Sidechain | 346/1608 (22%) | 236/1024 (23%) | 109/500 (22%)   | 1/84 (1%)       |
| Aromatic  | 34/148 (23%)   | 17/68 (25%)    | 17/80 (21%)     | 0/0 (—%)        |
| Overall   | 611/2696 (23%) | 347/1472 (24%) | 218/956 (23%)   | 46/268 (17%)    |

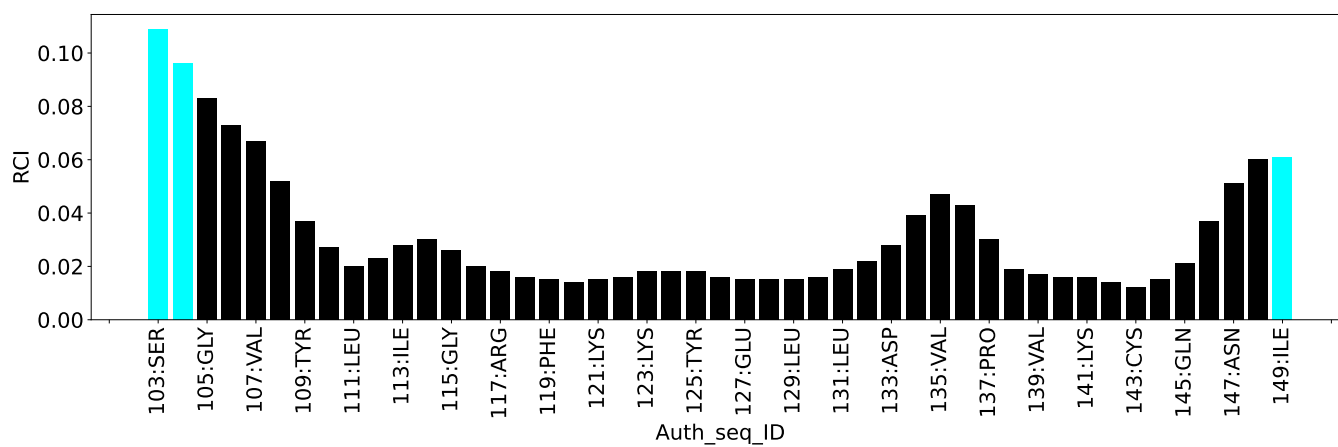
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

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

| Description                                              | Value |
|----------------------------------------------------------|-------|
| Total distance restraints                                | 1473  |
| Intra-residue ( $ i-j =0$ )                              | 300   |
| Sequential ( $ i-j =1$ )                                 | 322   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 293   |
| Long range ( $ i-j \geq 5$ )                             | 38    |
| Inter-chain                                              | 480   |
| Hydrogen bond restraints                                 | 40    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 106   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 8.4   |
| Number of long range restraints per residue <sup>1</sup> | 0.2   |

<sup>1</sup>Long 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)  | 25.8                                   | 0.2     |
| 0.2-0.5 (Medium) | 6.8                                    | 0.41    |
| >0.5 (Large)     | None                                   | None    |

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

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation. There are no dihedral-angle violations

## 9 Distance violation analysis ⓘ

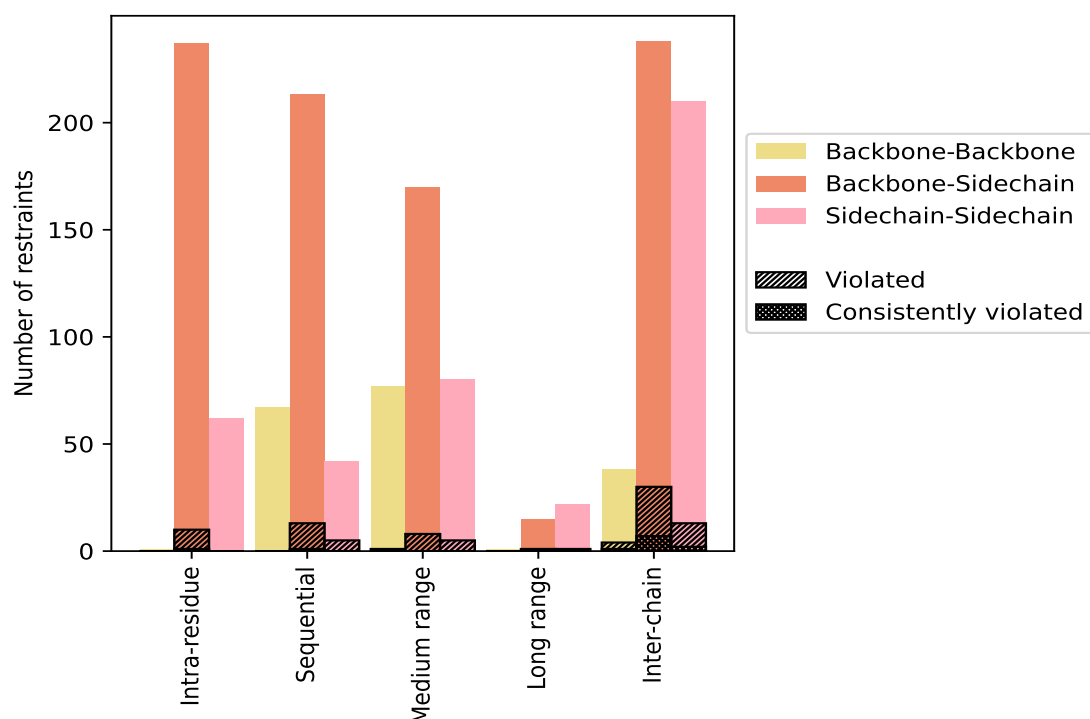
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>300</b>  | <b>20.4</b>    | <b>10</b>             | <b>3.3</b>     | <b>0.7</b>     | <b>1</b>                           | <b>0.3</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 1           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 237         | 16.1           | 10                    | 4.2            | 0.7            | 1                                  | 0.4            | 0.1            |
| Sidechain-Sidechain                                                         | 62          | 4.2            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>322</b>  | <b>21.9</b>    | <b>18</b>             | <b>5.6</b>     | <b>1.2</b>     | <b>1</b>                           | <b>0.3</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 67          | 4.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 213         | 14.5           | 13                    | 6.1            | 0.9            | 1                                  | 0.5            | 0.1            |
| Sidechain-Sidechain                                                         | 42          | 2.9            | 5                     | 11.9           | 0.3            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>293</b>  | <b>19.9</b>    | <b>12</b>             | <b>4.1</b>     | <b>0.8</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 77          | 5.2            | 1                     | 1.3            | 0.1            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 136         | 9.2            | 6                     | 4.4            | 0.4            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 80          | 5.4            | 5                     | 6.2            | 0.3            | 0                                  | 0.0            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>38</b>   | <b>2.6</b>     | <b>2</b>              | <b>5.3</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 1           | 0.1            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 15          | 1.0            | 1                     | 6.7            | 0.1            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 22          | 1.5            | 1                     | 4.5            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Inter-chain</b>                                                          | <b>480</b>  | <b>32.6</b>    | <b>47</b>             | <b>9.8</b>     | <b>3.2</b>     | <b>10</b>                          | <b>2.1</b>     | <b>0.7</b>     |
| Backbone-Backbone                                                           | 38          | 2.6            | 4                     | 10.5           | 0.3            | 1                                  | 2.6            | 0.1            |
| Backbone-Sidechain                                                          | 232         | 15.8           | 30                    | 12.9           | 2.0            | 7                                  | 3.0            | 0.5            |
| Sidechain-Sidechain                                                         | 210         | 14.3           | 13                    | 6.2            | 0.9            | 2                                  | 1.0            | 0.1            |
| <b>Hydrogen bond</b>                                                        | <b>40</b>   | <b>2.7</b>     | <b>2</b>              | <b>5.0</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>1473</b> | <b>100.0</b>   | <b>91</b>             | <b>6.2</b>     | <b>6.2</b>     | <b>12</b>                          | <b>0.8</b>     | <b>0.8</b>     |
| Backbone-Backbone                                                           | 184         | 12.5           | 5                     | 2.7            | 0.3            | 1                                  | 0.5            | 0.1            |
| Backbone-Sidechain                                                          | 873         | 59.3           | 62                    | 7.1            | 4.2            | 9                                  | 1.0            | 0.6            |
| Sidechain-Sidechain                                                         | 416         | 28.2           | 24                    | 5.8            | 1.6            | 2                                  | 0.5            | 0.1            |

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

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



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

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

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

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 1        | 3                    | 3               | 4               | 0               | 23              | 33    | 0.16     | 0.41    | 0.07                | 0.14       |
| 2        | 2                    | 5               | 5               | 0               | 20              | 32    | 0.17     | 0.31    | 0.06                | 0.16       |
| 3        | 3                    | 4               | 7               | 0               | 25              | 39    | 0.16     | 0.35    | 0.06                | 0.15       |
| 4        | 4                    | 5               | 4               | 0               | 21              | 34    | 0.16     | 0.36    | 0.06                | 0.15       |
| 5        | 4                    | 8               | 4               | 0               | 21              | 37    | 0.17     | 0.36    | 0.06                | 0.14       |
| 6        | 4                    | 5               | 3               | 1               | 24              | 37    | 0.16     | 0.41    | 0.06                | 0.13       |
| 7        | 3                    | 6               | 4               | 0               | 26              | 39    | 0.15     | 0.38    | 0.06                | 0.14       |
| 8        | 4                    | 6               | 5               | 0               | 21              | 36    | 0.16     | 0.38    | 0.06                | 0.15       |
| 9        | 3                    | 5               | 6               | 1               | 20              | 35    | 0.16     | 0.35    | 0.06                | 0.14       |
| 10       | 3                    | 7               | 4               | 0               | 22              | 36    | 0.16     | 0.34    | 0.06                | 0.14       |

*Continued on next page...*

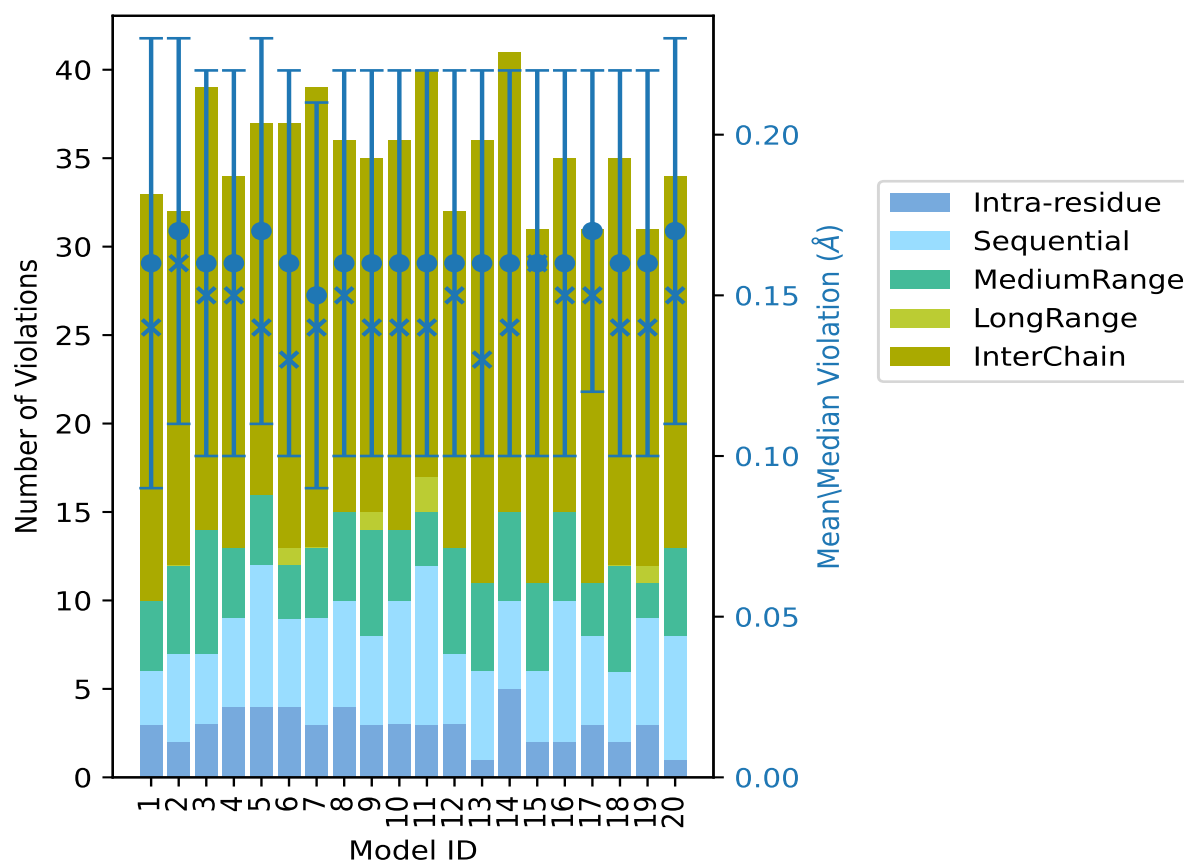
Continued from previous page...

| Model ID | Number of violations |                 |                 |                 |                 |       | Mean (Å) | Max (Å) | SD <sup>6</sup> (Å) | Median (Å) |
|----------|----------------------|-----------------|-----------------|-----------------|-----------------|-------|----------|---------|---------------------|------------|
|          | IR <sup>1</sup>      | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total |          |         |                     |            |
| 11       | 3                    | 9               | 3               | 2               | 23              | 40    | 0.16     | 0.41    | 0.06                | 0.14       |
| 12       | 3                    | 4               | 6               | 0               | 19              | 32    | 0.16     | 0.4     | 0.06                | 0.15       |
| 13       | 1                    | 5               | 5               | 0               | 25              | 36    | 0.16     | 0.36    | 0.06                | 0.13       |
| 14       | 5                    | 5               | 5               | 0               | 26              | 41    | 0.16     | 0.36    | 0.06                | 0.14       |
| 15       | 2                    | 4               | 5               | 0               | 20              | 31    | 0.16     | 0.34    | 0.06                | 0.16       |
| 16       | 2                    | 8               | 5               | 0               | 20              | 35    | 0.16     | 0.34    | 0.06                | 0.15       |
| 17       | 3                    | 5               | 3               | 0               | 20              | 31    | 0.17     | 0.31    | 0.05                | 0.15       |
| 18       | 2                    | 4               | 6               | 0               | 23              | 35    | 0.16     | 0.36    | 0.06                | 0.14       |
| 19       | 3                    | 6               | 2               | 1               | 19              | 31    | 0.16     | 0.39    | 0.06                | 0.14       |
| 20       | 1                    | 7               | 5               | 0               | 21              | 34    | 0.17     | 0.32    | 0.06                | 0.15       |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard 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

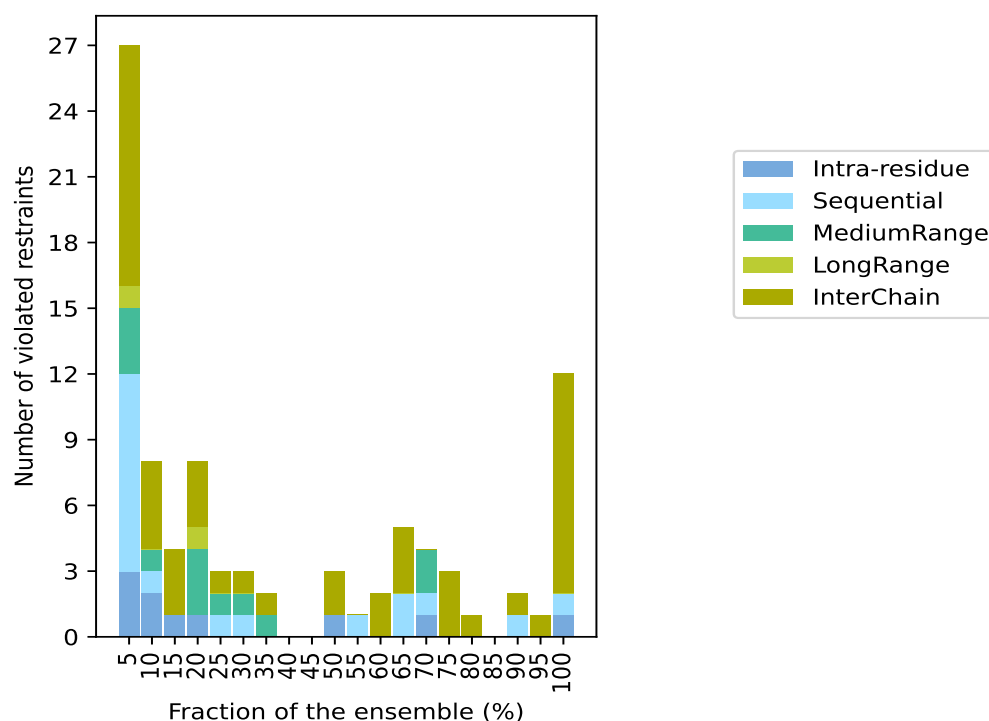
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1344(IR:290, SQ:304, MR:281, LR:36, IC:433) restraints are not violated in the ensemble.

| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| IR <sup>1</sup>               | SQ <sup>2</sup> | MR <sup>3</sup> | LR <sup>4</sup> | IC <sup>5</sup> | Total | Count <sup>6</sup>       | %     |
| 3                             | 9               | 3               | 1               | 11              | 27    | 1                        | 5.0   |
| 2                             | 1               | 1               | 0               | 4               | 8     | 2                        | 10.0  |
| 1                             | 0               | 0               | 0               | 3               | 4     | 3                        | 15.0  |
| 1                             | 0               | 3               | 1               | 3               | 8     | 4                        | 20.0  |
| 0                             | 1               | 1               | 0               | 1               | 3     | 5                        | 25.0  |
| 0                             | 1               | 1               | 0               | 1               | 3     | 6                        | 30.0  |
| 0                             | 0               | 1               | 0               | 1               | 2     | 7                        | 35.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 8                        | 40.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 9                        | 45.0  |
| 1                             | 0               | 0               | 0               | 2               | 3     | 10                       | 50.0  |
| 0                             | 1               | 0               | 0               | 0               | 1     | 11                       | 55.0  |
| 0                             | 0               | 0               | 0               | 2               | 2     | 12                       | 60.0  |
| 0                             | 2               | 0               | 0               | 3               | 5     | 13                       | 65.0  |
| 1                             | 1               | 2               | 0               | 0               | 4     | 14                       | 70.0  |
| 0                             | 0               | 0               | 0               | 3               | 3     | 15                       | 75.0  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 16                       | 80.0  |
| 0                             | 0               | 0               | 0               | 0               | 0     | 17                       | 85.0  |
| 0                             | 1               | 0               | 0               | 1               | 2     | 18                       | 90.0  |
| 0                             | 0               | 0               | 0               | 1               | 1     | 19                       | 95.0  |
| 1                             | 1               | 0               | 0               | 10              | 12    | 20                       | 100.0 |

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints,

<sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

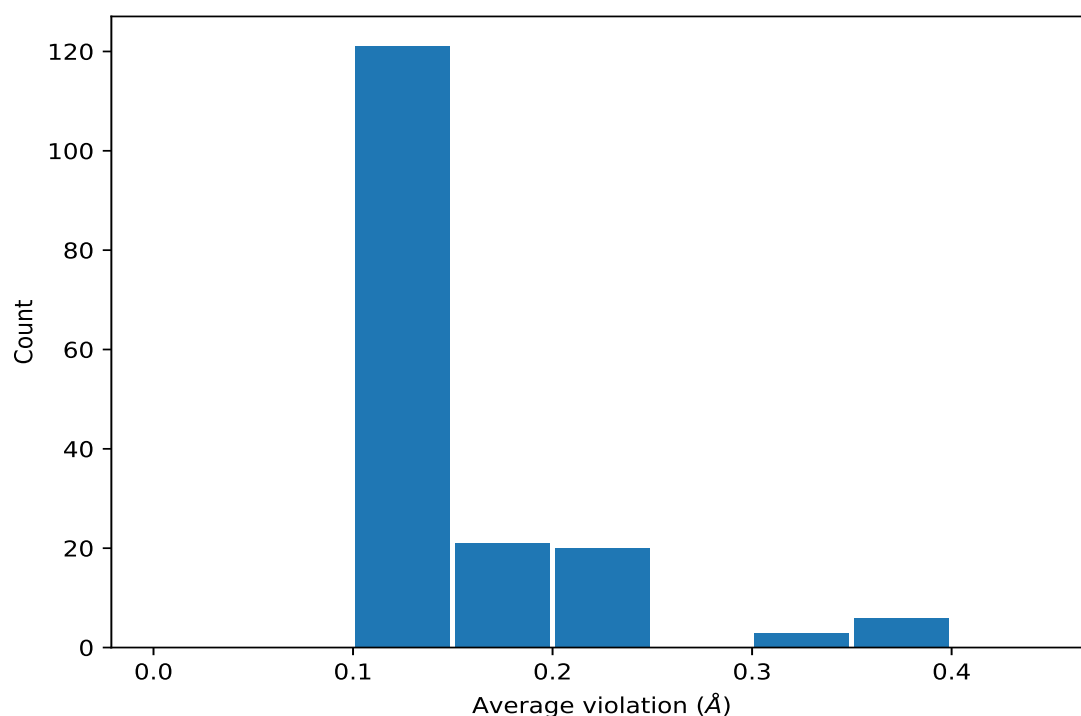
### 9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



## 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 <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 20                  | 0.36     | 0.03                | 0.36       |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 20                  | 0.31     | 0.02                | 0.31       |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 20                  | 0.31     | 0.02                | 0.31       |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 20                  | 0.31     | 0.02                | 0.31       |
| (1,1063) | 1:134:A:TYR:HE1 | 1:339:C:VAL:HG21 | 20                  | 0.23     | 0.03                | 0.23       |
| (1,1063) | 1:134:A:TYR:HE1 | 1:339:C:VAL:HG22 | 20                  | 0.23     | 0.03                | 0.23       |
| (1,1063) | 1:134:A:TYR:HE1 | 1:339:C:VAL:HG23 | 20                  | 0.23     | 0.03                | 0.23       |
| (1,1063) | 1:134:A:TYR:HE2 | 1:339:C:VAL:HG21 | 20                  | 0.23     | 0.03                | 0.23       |
| (1,1063) | 1:134:A:TYR:HE2 | 1:339:C:VAL:HG22 | 20                  | 0.23     | 0.03                | 0.23       |
| (1,1063) | 1:134:A:TYR:HE2 | 1:339:C:VAL:HG23 | 20                  | 0.23     | 0.03                | 0.23       |
| (1,732)  | 1:122:A:VAL:H   | 1:229:B:LEU:HD21 | 20                  | 0.22     | 0.02                | 0.22       |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 20                  | 0.22     | 0.02                | 0.22       |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 20                  | 0.22     | 0.02                | 0.22       |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 20                  | 0.22     | 0.01                | 0.22       |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 20                  | 0.22     | 0.01                | 0.22       |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 20                  | 0.22     | 0.01                | 0.22       |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 20                  | 0.21     | 0.03                | 0.21       |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 20                  | 0.21     | 0.03                | 0.21       |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 20                  | 0.21     | 0.03                | 0.21       |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 20                  | 0.2      | 0.04                | 0.2        |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 20                  | 0.2      | 0.04                | 0.2        |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 20                  | 0.2      | 0.03                | 0.19       |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 20                  | 0.2      | 0.03                | 0.19       |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 20                  | 0.2      | 0.03                | 0.19       |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 20                  | 0.18     | 0.03                | 0.18       |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 20                  | 0.18     | 0.03                | 0.18       |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 20                  | 0.16     | 0.02                | 0.17       |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 20                  | 0.16     | 0.03                | 0.16       |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 20                  | 0.15     | 0.02                | 0.15       |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 19                  | 0.17     | 0.03                | 0.17       |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 18                  | 0.14     | 0.03                | 0.14       |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 18                  | 0.14     | 0.03                | 0.14       |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 18                  | 0.13     | 0.01                | 0.13       |
| (1,232)  | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 18                  | 0.12     | 0.01                | 0.12       |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 16                  | 0.17     | 0.03                | 0.18       |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 16                  | 0.17     | 0.03                | 0.18       |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 16                  | 0.17     | 0.03                | 0.18       |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 16                  | 0.17     | 0.03                | 0.18       |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 16                  | 0.17     | 0.03                | 0.18       |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 16                  | 0.17     | 0.03                | 0.18       |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 15                  | 0.13     | 0.02                | 0.13       |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 15                  | 0.13     | 0.02                | 0.12       |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 15                  | 0.13     | 0.02                | 0.12       |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 15                  | 0.13     | 0.02                | 0.12       |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 15                  | 0.13     | 0.02                | 0.12       |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 15                  | 0.13     | 0.02                | 0.12       |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 15                  | 0.13     | 0.02                | 0.12       |
| (1,321)  | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 15                  | 0.12     | 0.02                | 0.12       |
| (1,321)  | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 15                  | 0.12     | 0.02                | 0.12       |
| (1,321)  | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 15                  | 0.12     | 0.02                | 0.12       |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 14                  | 0.16     | 0.01                | 0.17       |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 14                  | 0.16     | 0.01                | 0.17       |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 14                  | 0.16     | 0.03                | 0.16       |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 14                  | 0.16     | 0.03                | 0.16       |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 14                  | 0.16     | 0.03                | 0.16       |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 14                  | 0.16     | 0.03                | 0.16       |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 14                  | 0.16     | 0.03                | 0.16       |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 14                  | 0.16     | 0.03                | 0.16       |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 14                  | 0.15     | 0.01                | 0.15       |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 14                  | 0.14     | 0.03                | 0.13       |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 14                  | 0.14     | 0.03                | 0.13       |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 13                  | 0.16     | 0.04                | 0.14       |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 13                  | 0.16     | 0.04                | 0.14       |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 13                  | 0.15     | 0.03                | 0.14       |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 13                  | 0.15     | 0.03                | 0.14       |
| (1,657)  | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 13                  | 0.13     | 0.02                | 0.12       |
| (1,657)  | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 13                  | 0.13     | 0.02                | 0.12       |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 13                  | 0.13     | 0.01                | 0.13       |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 13                  | 0.13     | 0.01                | 0.13       |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 13                  | 0.13     | 0.01                | 0.13       |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 13                  | 0.13     | 0.01                | 0.13       |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 13                  | 0.13     | 0.01                | 0.13       |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 13                  | 0.13     | 0.01                | 0.13       |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 13                  | 0.12     | 0.02                | 0.12       |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 13                  | 0.12     | 0.02                | 0.12       |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 12                  | 0.12     | 0.01                | 0.13       |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 12                  | 0.12     | 0.01                | 0.12       |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 12                  | 0.12     | 0.01                | 0.12       |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 12                  | 0.12     | 0.01                | 0.12       |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 11                  | 0.12     | 0.02                | 0.12       |
| (1,465)  | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 10                  | 0.14     | 0.03                | 0.14       |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 10                  | 0.14     | 0.02                | 0.14       |
| (1,139)  | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 10                  | 0.13     | 0.01                | 0.14       |
| (1,139)  | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 10                  | 0.13     | 0.01                | 0.14       |
| (1,139)  | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 10                  | 0.13     | 0.01                | 0.14       |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 10                  | 0.11     | 0.01                | 0.11       |
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H    | 7                   | 0.13     | 0.02                | 0.13       |
| (1,354)  | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 7                   | 0.12     | 0.01                | 0.11       |
| (1,354)  | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 7                   | 0.12     | 0.01                | 0.11       |
| (1,354)  | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 7                   | 0.12     | 0.01                | 0.11       |
| (1,87)   | 1:107:A:VAL:H    | 1:109:A:TYR:HE1  | 6                   | 0.12     | 0.02                | 0.11       |
| (1,87)   | 1:107:A:VAL:H    | 1:109:A:TYR:HE2  | 6                   | 0.12     | 0.02                | 0.11       |
| (1,1298) | 1:143:A:CYS:HB2  | 1:144:A:CYS:HA   | 6                   | 0.12     | 0.01                | 0.11       |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,122)  | 1:108:A:VAL:HG11 | 1:212:B:ASN:HA   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,122)  | 1:108:A:VAL:HG12 | 1:212:B:ASN:HA   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,122)  | 1:108:A:VAL:HG13 | 1:212:B:ASN:HA   | 6                   | 0.11     | 0.01                | 0.11       |
| (1,56)   | 1:106:A:ASP:HB3  | 1:214:B:ARG:HE   | 5                   | 0.13     | 0.02                | 0.14       |
| (1,1103) | 1:135:A:VAL:HG11 | 1:136:A:GLN:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1103) | 1:135:A:VAL:HG12 | 1:136:A:GLN:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1103) | 1:135:A:VAL:HG13 | 1:136:A:GLN:HA   | 5                   | 0.11     | 0.01                | 0.11       |
| (1,594)  | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,594)  | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,594)  | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,594)  | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG21 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,594)  | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG22 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,594)  | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG23 | 5                   | 0.11     | 0.01                | 0.11       |
| (1,1334) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3  | 4                   | 0.14     | 0.06                | 0.11       |
| (1,298)  | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE1  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,298)  | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE2  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,298)  | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE1  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,298)  | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE2  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,298)  | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE1  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,298)  | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE2  | 4                   | 0.12     | 0.02                | 0.12       |
| (1,315)  | 1:111:A:LEU:HD21 | 1:226:B:LYS:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,315)  | 1:111:A:LEU:HD22 | 1:226:B:LYS:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,315)  | 1:111:A:LEU:HD23 | 1:226:B:LYS:HA   | 4                   | 0.12     | 0.01                | 0.12       |
| (1,611)  | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,611)  | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,611)  | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE2  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,611)  | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE3  | 4                   | 0.12     | 0.01                | 0.12       |
| (1,224)  | 1:110:A:THR:HG21 | 1:112:A:ASN:HA   | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,224)  | 1:110:A:THR:HG22 | 1:112:A:ASN:HA   | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,224)  | 1:110:A:THR:HG23 | 1:112:A:ASN:HA   | 4                   | 0.12     | 0.0                 | 0.12       |
| (1,1139) | 1:136:A:GLN:HG2  | 1:139:A:VAL:HB   | 4                   | 0.12     | 0.01                | 0.11       |
| (1,1139) | 1:136:A:GLN:HG3  | 1:139:A:VAL:HB   | 4                   | 0.12     | 0.01                | 0.11       |
| (1,404)  | 1:113:A:ILE:HD11 | 1:226:B:LYS:HA   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,404)  | 1:113:A:ILE:HD12 | 1:226:B:LYS:HA   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,404)  | 1:113:A:ILE:HD13 | 1:226:B:LYS:HA   | 4                   | 0.11     | 0.01                | 0.11       |
| (1,815)  | 1:125:A:TYR:HE1  | 1:132:A:LEU:HG   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,815)  | 1:125:A:TYR:HE2  | 1:132:A:LEU:HG   | 4                   | 0.11     | 0.0                 | 0.11       |
| (1,1082) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD2  | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1082) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD2  | 3                   | 0.14     | 0.0                 | 0.14       |
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD2  | 3                   | 0.14     | 0.04                | 0.11       |
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3  | 3                   | 0.14     | 0.04                | 0.11       |
| (1,728)  | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD11 | 3                   | 0.12     | 0.01                | 0.13       |

*Continued on next page...*

Continued from previous page...

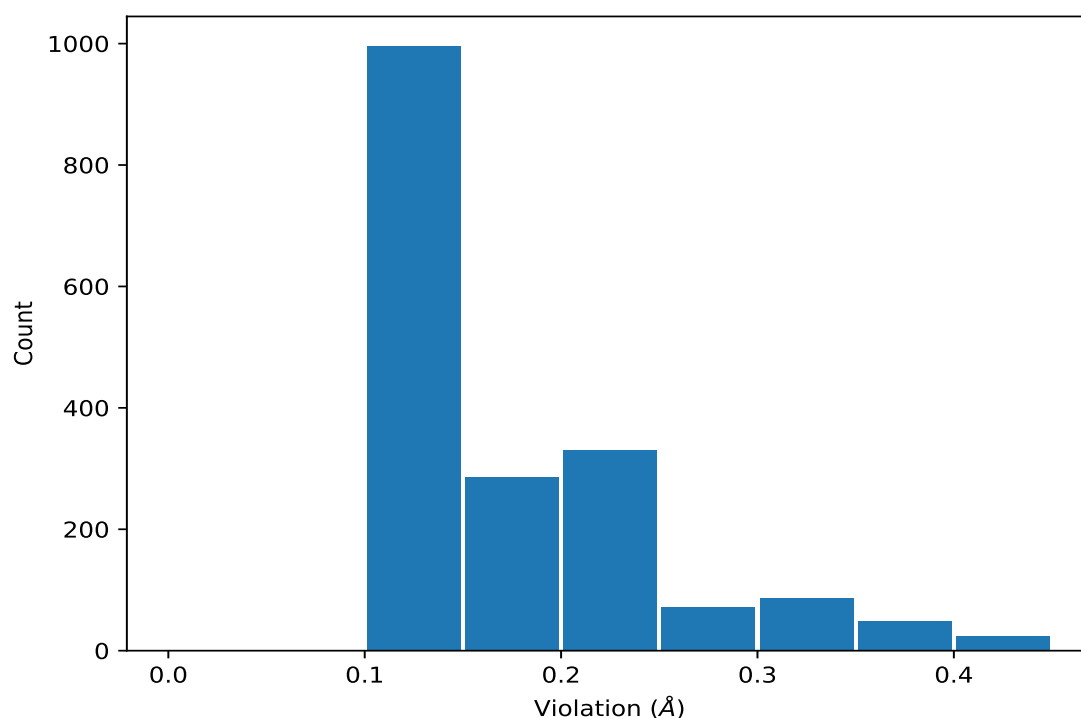
| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,728)  | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD12 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,728)  | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD13 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,728)  | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD11 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,728)  | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD12 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,728)  | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD13 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,728)  | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD11 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,728)  | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD12 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,728)  | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD13 | 3                   | 0.12     | 0.01                | 0.13       |
| (1,675)  | 1:121:A:LYS:H    | 1:229:B:LEU:HD11 | 3                   | 0.11     | 0.01                | 0.12       |
| (1,675)  | 1:121:A:LYS:H    | 1:229:B:LEU:HD12 | 3                   | 0.11     | 0.01                | 0.12       |
| (1,675)  | 1:121:A:LYS:H    | 1:229:B:LEU:HD13 | 3                   | 0.11     | 0.01                | 0.12       |
| (1,421)  | 1:114:A:ARG:H    | 1:114:A:ARG:HD2  | 2                   | 0.13     | 0.02                | 0.13       |
| (1,743)  | 1:123:A:LYS:H    | 1:123:A:LYS:HE2  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,743)  | 1:123:A:LYS:H    | 1:123:A:LYS:HE3  | 2                   | 0.13     | 0.01                | 0.13       |
| (1,1003) | 1:131:A:LEU:HA   | 1:343:C:CYS:HA   | 2                   | 0.12     | 0.01                | 0.12       |
| (1,1291) | 1:142:A:ALA:HB1  | 1:146:A:ARG:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1291) | 1:142:A:ALA:HB2  | 1:146:A:ARG:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,1291) | 1:142:A:ALA:HB3  | 1:146:A:ARG:H    | 2                   | 0.12     | 0.0                 | 0.12       |
| (1,281)  | 1:111:A:LEU:HD21 | 1:219:B:PHE:HA   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,281)  | 1:111:A:LEU:HD22 | 1:219:B:PHE:HA   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,281)  | 1:111:A:LEU:HD23 | 1:219:B:PHE:HA   | 2                   | 0.11     | 0.01                | 0.11       |
| (1,676)  | 1:121:A:LYS:HA   | 1:229:B:LEU:HD11 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,676)  | 1:121:A:LYS:HA   | 1:229:B:LEU:HD12 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,676)  | 1:121:A:LYS:HA   | 1:229:B:LEU:HD13 | 2                   | 0.11     | 0.01                | 0.11       |
| (1,278)  | 1:111:A:LEU:H    | 1:213:B:ILE:HD11 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,278)  | 1:111:A:LEU:H    | 1:213:B:ILE:HD12 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,278)  | 1:111:A:LEU:H    | 1:213:B:ILE:HD13 | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,517)  | 1:117:A:ARG:H    | 1:118:A:LYS:HE2  | 2                   | 0.1      | 0.0                 | 0.1        |
| (1,517)  | 1:117:A:ARG:H    | 1:118:A:LYS:HE3  | 2                   | 0.1      | 0.0                 | 0.1        |

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

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

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



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

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

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 1        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 1        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 1        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 1        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 1        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 1        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 6        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 6        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 6        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 6        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 6        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 6        | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 11       | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 11       | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 11       | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 11       | 0.41          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 11       | 0.41          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 11       | 0.41          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 12       | 0.4           |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 12       | 0.4           |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 12       | 0.4           |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 12       | 0.4           |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 12       | 0.4           |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 12       | 0.4           |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 19       | 0.39          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 19       | 0.39          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 19       | 0.39          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 19       | 0.39          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 19       | 0.39          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 19       | 0.39          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 7        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 7        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 7        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 7        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 7        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 7        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 8        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 8        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 8        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 8        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 8        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 8        | 0.38          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 4        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 4        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 4        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 4        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 4        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 4        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 5        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 5        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 5        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 5        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 5        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 5        | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 13       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 13       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 13       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 13       | 0.36          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 13       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 13       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 14       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 14       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 14       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 14       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 14       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 14       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 18       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 18       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 18       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 18       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 18       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 18       | 0.36          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 3        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 3        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 3        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 3        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 3        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 3        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 9        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 9        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 9        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 9        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 9        | 0.35          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 9        | 0.35          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 10       | 0.34          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 10       | 0.34          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 10       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 15       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 15       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 15       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 15       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 15       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 15       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 16       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 16       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 16       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 16       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 16       | 0.34          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 16       | 0.34          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 7        | 0.33          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 7        | 0.33          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 7        | 0.33          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 10       | 0.33          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 10       | 0.33          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 10       | 0.33          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 10       | 0.33          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 10       | 0.33          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 10       | 0.33          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 1        | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 1        | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 1        | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 5        | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 5        | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 5        | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 15       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 15       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 15       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 19       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 19       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 19       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 20       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 20       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 20       | 0.32          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 20       | 0.32          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 20       | 0.32          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 20       | 0.32          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 20       | 0.32          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 20       | 0.32          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 20       | 0.32          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 4        | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 4        | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 4        | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 6        | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 6        | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 6        | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 11       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 11       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 11       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 12       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 12       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 12       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 13       | 0.31          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 13       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 13       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 16       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 16       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 16       | 0.31          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 2        | 0.31          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 2        | 0.31          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 2        | 0.31          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 2        | 0.31          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 2        | 0.31          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 2        | 0.31          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG11 | 17       | 0.31          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG12 | 17       | 0.31          |
| (1,1061) | 1:134:A:TYR:HD1 | 1:339:C:VAL:HG13 | 17       | 0.31          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG11 | 17       | 0.31          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG12 | 17       | 0.31          |
| (1,1061) | 1:134:A:TYR:HD2 | 1:339:C:VAL:HG13 | 17       | 0.31          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 8        | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 8        | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 8        | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 14       | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 14       | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 14       | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 17       | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 17       | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 17       | 0.3           |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 2        | 0.29          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 2        | 0.29          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 2        | 0.29          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 3        | 0.29          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 3        | 0.29          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 3        | 0.29          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 18       | 0.28          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 18       | 0.28          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 18       | 0.28          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG11 | 9        | 0.27          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG12 | 9        | 0.27          |
| (1,1106) | 1:135:A:VAL:H   | 1:335:C:VAL:HG13 | 9        | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1 | 1:339:C:VAL:HG21 | 14       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1 | 1:339:C:VAL:HG22 | 14       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1 | 1:339:C:VAL:HG23 | 14       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2 | 1:339:C:VAL:HG21 | 14       | 0.27          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 14       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 14       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 17       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 17       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 17       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 17       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 17       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 17       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 20       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 20       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 20       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 20       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 20       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 20       | 0.27          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 3        | 0.27          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 3        | 0.27          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 3        | 0.27          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 13       | 0.27          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 13       | 0.27          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 13       | 0.27          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 7        | 0.26          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 7        | 0.26          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 7        | 0.26          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 7        | 0.26          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 7        | 0.26          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 7        | 0.26          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 20       | 0.26          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 20       | 0.26          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 20       | 0.26          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 12       | 0.26          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 12       | 0.26          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 8        | 0.25          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 8        | 0.25          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 8        | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 2        | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 2        | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 2        | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 11       | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 11       | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 11       | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 17       | 0.25          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 17       | 0.25          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 17       | 0.25          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 2        | 0.25          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 2        | 0.25          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 2        | 0.25          |
| (1,1334) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3  | 4        | 0.24          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 20       | 0.24          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 20       | 0.24          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 3        | 0.24          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 3        | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 8        | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 8        | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 8        | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 8        | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 8        | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 8        | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 10       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 10       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 10       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 10       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 10       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 10       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 16       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 16       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 16       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 16       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 16       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 16       | 0.24          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 5        | 0.24          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 5        | 0.24          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 5        | 0.24          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 18       | 0.24          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 18       | 0.24          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 18       | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 3        | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 3        | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 3        | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 10       | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 10       | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 10       | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 18       | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 18       | 0.24          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 18       | 0.24          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 14       | 0.24          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 14       | 0.24          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 14       | 0.24          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 1        | 0.24          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 1        | 0.24          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 5        | 0.24          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 5        | 0.24          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 19       | 0.24          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 19       | 0.24          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 1        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 1        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 1        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 1        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 1        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 1        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 2        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 2        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 2        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 2        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 2        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 2        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 4        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 4        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 4        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 4        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 4        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 4        | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 12       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 12       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 12       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 12       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 12       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 12       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 15       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 15       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 15       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 15       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 15       | 0.23          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 15       | 0.23          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 9        | 0.23          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 9        | 0.23          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 9        | 0.23          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 10       | 0.23          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 10       | 0.23          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 10       | 0.23          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 10       | 0.23          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 10       | 0.23          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 10       | 0.23          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 2        | 0.23          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 10       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 10       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 10       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 11       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 11       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 11       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 12       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 12       | 0.23          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 12       | 0.23          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 9        | 0.23          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 9        | 0.23          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 11       | 0.23          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 11       | 0.23          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 13       | 0.23          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 13       | 0.23          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 14       | 0.22          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 14       | 0.22          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 14       | 0.22          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 14       | 0.22          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 5        | 0.22          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 5        | 0.22          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 7        | 0.22          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 7        | 0.22          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 14       | 0.22          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 14       | 0.22          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 17       | 0.22          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 17       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 2        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 2        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 2        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 7        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 7        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 7        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 9        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 9        | 0.22          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 9        | 0.22          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 13       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 13       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 13       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 15       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 15       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 15       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 16       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 16       | 0.22          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 16       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 1        | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 1        | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 1        | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 12       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 12       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 12       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 14       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 14       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 14       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 16       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 16       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 16       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 19       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 19       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 19       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 20       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 20       | 0.22          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 20       | 0.22          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 16       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 8        | 0.22          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 8        | 0.22          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 8        | 0.22          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 9        | 0.22          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 9        | 0.22          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 9        | 0.22          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 13       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 13       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 13       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 17       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 17       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 17       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 20       | 0.22          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 20       | 0.22          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 20       | 0.22          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 2        | 0.22          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 2        | 0.22          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 4        | 0.22          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 4        | 0.22          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 3        | 0.21          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 3        | 0.21          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 5        | 0.21          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 5        | 0.21          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 5        | 0.21          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 5        | 0.21          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 5        | 0.21          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 5        | 0.21          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 16       | 0.21          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 16       | 0.21          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 16       | 0.21          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 16       | 0.21          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 16       | 0.21          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 16       | 0.21          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 19       | 0.21          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 19       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 5        | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 5        | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 5        | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 5        | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 5        | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 5        | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 13       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 13       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 13       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 13       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 13       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 13       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 18       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 18       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 18       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 18       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 18       | 0.21          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 18       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 1        | 0.21          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 1        | 0.21          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 1        | 0.21          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 6        | 0.21          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 6        | 0.21          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 6        | 0.21          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 10       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 10       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 10       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 11       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 11       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 11       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 20       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 20       | 0.21          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 20       | 0.21          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 5        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 5        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 5        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 6        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 6        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 6        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 7        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 7        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 7        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 9        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 9        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 9        | 0.21          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 11       | 0.21          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 11       | 0.21          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 11       | 0.21          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 19       | 0.21          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 19       | 0.21          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 19       | 0.21          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 5        | 0.21          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 5        | 0.21          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 5        | 0.21          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 8        | 0.21          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 8        | 0.21          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 8        | 0.21          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 13       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 1        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 1        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 1        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 3        | 0.21          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 3        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 3        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 5        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 5        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 5        | 0.21          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 15       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 15       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 15       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 18       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 18       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 18       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 19       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 19       | 0.21          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 19       | 0.21          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 20       | 0.21          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 20       | 0.21          |
| (1,190)  | 1:109:A:TYR:HD1  | 1:216:B:LYS:HE2  | 13       | 0.21          |
| (1,190)  | 1:109:A:TYR:HD1  | 1:216:B:LYS:HE3  | 13       | 0.21          |
| (1,190)  | 1:109:A:TYR:HD2  | 1:216:B:LYS:HE2  | 13       | 0.21          |
| (1,190)  | 1:109:A:TYR:HD2  | 1:216:B:LYS:HE3  | 13       | 0.21          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 11       | 0.2           |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 11       | 0.2           |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 8        | 0.2           |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 8        | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 6        | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 6        | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 6        | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 6        | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 6        | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 6        | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 11       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 11       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 11       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 11       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 11       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 11       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 19       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 19       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 19       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 19       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 19       | 0.2           |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 19       | 0.2           |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 5        | 0.2           |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 17       | 0.2           |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 17       | 0.2           |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 17       | 0.2           |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 4        | 0.2           |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 4        | 0.2           |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 6        | 0.2           |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 6        | 0.2           |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 4        | 0.2           |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 4        | 0.2           |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 4        | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 2        | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 2        | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 2        | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 2        | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 2        | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 2        | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 16       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 16       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 16       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 16       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 16       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 16       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 18       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 18       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 18       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 18       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 18       | 0.2           |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 18       | 0.2           |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 9        | 0.2           |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 10       | 0.2           |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 7        | 0.2           |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 7        | 0.2           |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 7        | 0.2           |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 16       | 0.2           |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 16       | 0.2           |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 16       | 0.2           |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 3        | 0.2           |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 3        | 0.2           |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 6        | 0.2           |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 6        | 0.2           |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 8        | 0.19          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 8        | 0.19          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 17       | 0.19          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 17       | 0.19          |
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD2  | 4        | 0.19          |
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3  | 4        | 0.19          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 11       | 0.19          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 11       | 0.19          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 11       | 0.19          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 11       | 0.19          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 11       | 0.19          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 11       | 0.19          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 8        | 0.19          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 8        | 0.19          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 6        | 0.19          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 6        | 0.19          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 10       | 0.19          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 10       | 0.19          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 3        | 0.19          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 3        | 0.19          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 3        | 0.19          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 3        | 0.19          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 3        | 0.19          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 3        | 0.19          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 9        | 0.19          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 8        | 0.19          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 8        | 0.19          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 8        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 1        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 1        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 1        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 2        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 2        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 2        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 3        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 3        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 3        | 0.19          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 10       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 10       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 10       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 12       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 12       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 12       | 0.19          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 17       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 17       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 17       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 18       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 18       | 0.19          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 18       | 0.19          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 4        | 0.19          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 8        | 0.19          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 8        | 0.19          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 8        | 0.19          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 8        | 0.19          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 8        | 0.19          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 8        | 0.19          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 4        | 0.19          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 5        | 0.19          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 15       | 0.19          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 4        | 0.19          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 4        | 0.19          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 4        | 0.19          |
| (1,300)  | 1:111:A:LEU:HD11 | 1:223:B:LYS:H    | 6        | 0.19          |
| (1,300)  | 1:111:A:LEU:HD12 | 1:223:B:LYS:H    | 6        | 0.19          |
| (1,300)  | 1:111:A:LEU:HD13 | 1:223:B:LYS:H    | 6        | 0.19          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 15       | 0.18          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 15       | 0.18          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 15       | 0.18          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 15       | 0.18          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 15       | 0.18          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 15       | 0.18          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 4        | 0.18          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 4        | 0.18          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 12       | 0.18          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 12       | 0.18          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 20       | 0.18          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 20       | 0.18          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG21 | 9        | 0.18          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG22 | 9        | 0.18          |
| (1,1063) | 1:134:A:TYR:HE1  | 1:339:C:VAL:HG23 | 9        | 0.18          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG21 | 9        | 0.18          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG22 | 9        | 0.18          |
| (1,1063) | 1:134:A:TYR:HE2  | 1:339:C:VAL:HG23 | 9        | 0.18          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 2        | 0.18          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 3        | 0.18          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 4        | 0.18          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 18       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 13       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 13       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 13       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 14       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 14       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 14       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 15       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 15       | 0.18          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 15       | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 6        | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 6        | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 6        | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 7        | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 7        | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 7        | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD21 | 15       | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD22 | 15       | 0.18          |
| (1,732)  | 1:122:A:VAL:H    | 1:229:B:LEU:HD23 | 15       | 0.18          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 5        | 0.18          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 10       | 0.18          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 12       | 0.18          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 15       | 0.18          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 18       | 0.18          |
| (1,465)  | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 3        | 0.18          |
| (1,465)  | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 11       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 1        | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 1        | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 1        | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 1        | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 1        | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 1        | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 11       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 11       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 11       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 11       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 11       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 11       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 17       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 17       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 17       | 0.18          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 17       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 17       | 0.18          |
| (1,453)  | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 17       | 0.18          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 3        | 0.18          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 3        | 0.17          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 18       | 0.17          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 20       | 0.17          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 20       | 0.17          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 16       | 0.17          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 2        | 0.17          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 2        | 0.17          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 9        | 0.17          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 9        | 0.17          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 9        | 0.17          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 9        | 0.17          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 16       | 0.17          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 16       | 0.17          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 19       | 0.17          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 19       | 0.17          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 6        | 0.17          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 13       | 0.17          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 20       | 0.17          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 4        | 0.17          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 4        | 0.17          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 4        | 0.17          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 15       | 0.17          |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 7        | 0.17          |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 7        | 0.17          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 7        | 0.17          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 7        | 0.17          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 7        | 0.17          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 7        | 0.17          |
| (1,657)  | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 20       | 0.17          |
| (1,657)  | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 20       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 2        | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 2        | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 3        | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 3        | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 8        | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 8        | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 10       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 10       | 0.17          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE2  | 14       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE3  | 14       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE2  | 15       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE3  | 15       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE2  | 16       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE3  | 16       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE2  | 17       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE3  | 17       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE2  | 18       | 0.17          |
| (1,610)  | 1:119:A:PHE:HZ  | 1:123:A:LYS:HE3  | 18       | 0.17          |
| (1,529)  | 1:118:A:LYS:H   | 1:118:A:LYS:HD3  | 2        | 0.17          |
| (1,529)  | 1:118:A:LYS:H   | 1:118:A:LYS:HD3  | 8        | 0.17          |
| (1,529)  | 1:118:A:LYS:H   | 1:118:A:LYS:HD3  | 16       | 0.17          |
| (1,529)  | 1:118:A:LYS:H   | 1:118:A:LYS:HD3  | 17       | 0.17          |
| (1,529)  | 1:118:A:LYS:H   | 1:118:A:LYS:HD3  | 19       | 0.17          |
| (1,481)  | 1:116:A:LYS:HE2 | 1:117:A:ARG:H    | 11       | 0.17          |
| (1,481)  | 1:116:A:LYS:HE3 | 1:117:A:ARG:H    | 11       | 0.17          |
| (1,465)  | 1:116:A:LYS:HA  | 1:116:A:LYS:HD2  | 8        | 0.17          |
| (1,453)  | 1:114:A:ARG:HD2 | 1:449:D:ILE:HG21 | 20       | 0.17          |
| (1,453)  | 1:114:A:ARG:HD2 | 1:449:D:ILE:HG22 | 20       | 0.17          |
| (1,453)  | 1:114:A:ARG:HD2 | 1:449:D:ILE:HG23 | 20       | 0.17          |
| (1,453)  | 1:114:A:ARG:HD3 | 1:449:D:ILE:HG21 | 20       | 0.17          |
| (1,453)  | 1:114:A:ARG:HD3 | 1:449:D:ILE:HG22 | 20       | 0.17          |
| (1,453)  | 1:114:A:ARG:HD3 | 1:449:D:ILE:HG23 | 20       | 0.17          |
| (1,437)  | 1:114:A:ARG:H   | 1:449:D:ILE:HA   | 6        | 0.17          |
| (1,437)  | 1:114:A:ARG:H   | 1:449:D:ILE:HA   | 7        | 0.17          |
| (1,437)  | 1:114:A:ARG:H   | 1:449:D:ILE:HA   | 14       | 0.17          |
| (1,228)  | 1:110:A:THR:HA  | 1:211:B:LEU:H    | 4        | 0.17          |
| (1,228)  | 1:110:A:THR:HA  | 1:211:B:LEU:H    | 12       | 0.17          |
| (1,228)  | 1:110:A:THR:HA  | 1:211:B:LEU:H    | 15       | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE1  | 8        | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE2  | 8        | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE1  | 14       | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE2  | 14       | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE1  | 15       | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE2  | 15       | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE1  | 18       | 0.17          |
| (1,210)  | 1:109:A:TYR:HA  | 1:219:B:PHE:HE2  | 18       | 0.17          |
| (1,1376) | 1:148:A:GLN:HG2 | 1:149:A:ILE:HB   | 2        | 0.16          |
| (1,1376) | 1:148:A:GLN:HG3 | 1:149:A:ILE:HB   | 2        | 0.16          |
| (1,1353) | 1:146:A:ARG:H   | 1:147:A:ASN:HB2  | 11       | 0.16          |
| (1,1353) | 1:146:A:ARG:H   | 1:147:A:ASN:HB3  | 11       | 0.16          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H   | 3        | 0.16          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2 | 14       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3 | 14       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2 | 14       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3 | 14       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2 | 14       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3 | 14       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2 | 17       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3 | 17       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2 | 17       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3 | 17       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2 | 17       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3 | 17       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2 | 20       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3 | 20       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2 | 20       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3 | 20       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2 | 20       | 0.16          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3 | 20       | 0.16          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3 | 3        | 0.16          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3 | 3        | 0.16          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA  | 1        | 0.16          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA  | 1        | 0.16          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA  | 2        | 0.16          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA  | 2        | 0.16          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA  | 15       | 0.16          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA  | 15       | 0.16          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB  | 10       | 0.16          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB  | 11       | 0.16          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB  | 12       | 0.16          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H   | 12       | 0.16          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H   | 12       | 0.16          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H   | 12       | 0.16          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H   | 19       | 0.16          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H   | 19       | 0.16          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H   | 19       | 0.16          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2 | 2        | 0.16          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2 | 3        | 0.16          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2 | 5        | 0.16          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2 | 9        | 0.16          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2 | 16       | 0.16          |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1 | 8        | 0.16          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 8        | 0.16          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 8        | 0.16          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 8        | 0.16          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 8        | 0.16          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 8        | 0.16          |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 15       | 0.16          |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 15       | 0.16          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 15       | 0.16          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 15       | 0.16          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 15       | 0.16          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 15       | 0.16          |
| (1,657)  | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 14       | 0.16          |
| (1,657)  | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 14       | 0.16          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 5        | 0.16          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 5        | 0.16          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 12       | 0.16          |
| (1,610)  | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 12       | 0.16          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 6        | 0.16          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 9        | 0.16          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 11       | 0.16          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 13       | 0.16          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 20       | 0.16          |
| (1,437)  | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 1        | 0.16          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 3        | 0.16          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 7        | 0.16          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 13       | 0.16          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 14       | 0.16          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 18       | 0.16          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 16       | 0.16          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 16       | 0.16          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 17       | 0.16          |
| (1,210)  | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 17       | 0.16          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 17       | 0.16          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 8        | 0.15          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 4        | 0.15          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 4        | 0.15          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 14       | 0.15          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 14       | 0.15          |
| (1,1372) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HA   | 5        | 0.15          |
| (1,1372) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HA   | 5        | 0.15          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 7        | 0.15          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 7        | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 18       | 0.15          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 18       | 0.15          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 7        | 0.15          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 7        | 0.15          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 7        | 0.15          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 7        | 0.15          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 7        | 0.15          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 7        | 0.15          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 13       | 0.15          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 13       | 0.15          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 13       | 0.15          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 13       | 0.15          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 13       | 0.15          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 13       | 0.15          |
| (1,1125) | 1:136:A:GLN:HB2  | 1:137:A:PRO:HD2  | 16       | 0.15          |
| (1,1125) | 1:136:A:GLN:HB2  | 1:137:A:PRO:HD3  | 16       | 0.15          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 7        | 0.15          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 7        | 0.15          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 5        | 0.15          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 5        | 0.15          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 18       | 0.15          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 18       | 0.15          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 1        | 0.15          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 16       | 0.15          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 17       | 0.15          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 14       | 0.15          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 14       | 0.15          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 14       | 0.15          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 12       | 0.15          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 12       | 0.15          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 20       | 0.15          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 20       | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 6        | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 6        | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 6        | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 6        | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 6        | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 6        | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 12       | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 12       | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 12       | 0.15          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 12       | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 12       | 0.15          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 12       | 0.15          |
| (1,737) | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 7        | 0.15          |
| (1,737) | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 10       | 0.15          |
| (1,737) | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 11       | 0.15          |
| (1,737) | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 18       | 0.15          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 14       | 0.15          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 14       | 0.15          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 14       | 0.15          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 14       | 0.15          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 14       | 0.15          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 14       | 0.15          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 2        | 0.15          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 2        | 0.15          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 11       | 0.15          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 11       | 0.15          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 12       | 0.15          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 12       | 0.15          |
| (1,610) | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 4        | 0.15          |
| (1,610) | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 4        | 0.15          |
| (1,610) | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 7        | 0.15          |
| (1,610) | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 7        | 0.15          |
| (1,529) | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 1        | 0.15          |
| (1,465) | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 10       | 0.15          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 3        | 0.15          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 3        | 0.15          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 3        | 0.15          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 3        | 0.15          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 3        | 0.15          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 3        | 0.15          |
| (1,437) | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 12       | 0.15          |
| (1,437) | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 20       | 0.15          |
| (1,421) | 1:114:A:ARG:H    | 1:114:A:ARG:HD2  | 14       | 0.15          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 6        | 0.15          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 6        | 0.15          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 6        | 0.15          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 17       | 0.15          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 17       | 0.15          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 17       | 0.15          |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE1  | 13       | 0.15          |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE2  | 13       | 0.15          |
| (1,298) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE1  | 13       | 0.15          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,298)  | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE2 | 13       | 0.15          |
| (1,298)  | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE1 | 13       | 0.15          |
| (1,298)  | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE2 | 13       | 0.15          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H   | 5        | 0.15          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H   | 8        | 0.15          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H   | 10       | 0.15          |
| (1,228)  | 1:110:A:THR:HA   | 1:211:B:LEU:H   | 16       | 0.15          |
| (1,87)   | 1:107:A:VAL:H    | 1:109:A:TYR:HE1 | 20       | 0.15          |
| (1,87)   | 1:107:A:VAL:H    | 1:109:A:TYR:HE2 | 20       | 0.15          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H   | 2        | 0.15          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H   | 16       | 0.15          |
| (1,56)   | 1:106:A:ASP:HB3  | 1:214:B:ARG:HE  | 7        | 0.15          |
| (1,56)   | 1:106:A:ASP:HB3  | 1:214:B:ARG:HE  | 19       | 0.15          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H   | 1        | 0.14          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H   | 12       | 0.14          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H   | 1        | 0.14          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H   | 3        | 0.14          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H   | 12       | 0.14          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H   | 16       | 0.14          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H   | 17       | 0.14          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2 | 14       | 0.14          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3 | 14       | 0.14          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2 | 16       | 0.14          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3 | 16       | 0.14          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2 | 19       | 0.14          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3 | 19       | 0.14          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H   | 19       | 0.14          |
| (1,1298) | 1:143:A:CYS:HB2  | 1:144:A:CYS:HA  | 5        | 0.14          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2 | 10       | 0.14          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3 | 10       | 0.14          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2 | 10       | 0.14          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3 | 10       | 0.14          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2 | 10       | 0.14          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3 | 10       | 0.14          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2 | 6        | 0.14          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2 | 6        | 0.14          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3 | 4        | 0.14          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3 | 4        | 0.14          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3 | 12       | 0.14          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3 | 12       | 0.14          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3 | 17       | 0.14          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3 | 17       | 0.14          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1082) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD2  | 8        | 0.14          |
| (1,1082) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD2  | 8        | 0.14          |
| (1,1082) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD2  | 14       | 0.14          |
| (1,1082) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD2  | 14       | 0.14          |
| (1,1082) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD2  | 19       | 0.14          |
| (1,1082) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD2  | 19       | 0.14          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 19       | 0.14          |
| (1,1009) | 1:131:A:LEU:HD21 | 1:344:C:CYS:H    | 4        | 0.14          |
| (1,1009) | 1:131:A:LEU:HD22 | 1:344:C:CYS:H    | 4        | 0.14          |
| (1,1009) | 1:131:A:LEU:HD23 | 1:344:C:CYS:H    | 4        | 0.14          |
| (1,993)  | 1:131:A:LEU:HG   | 1:335:C:VAL:H    | 7        | 0.14          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 9        | 0.14          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 9        | 0.14          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 18       | 0.14          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 18       | 0.14          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 2        | 0.14          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 3        | 0.14          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 11       | 0.14          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 12       | 0.14          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 19       | 0.14          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 19       | 0.14          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 19       | 0.14          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 19       | 0.14          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 19       | 0.14          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 19       | 0.14          |
| (1,743)  | 1:123:A:LYS:H    | 1:123:A:LYS:HE2  | 19       | 0.14          |
| (1,743)  | 1:123:A:LYS:H    | 1:123:A:LYS:HE3  | 19       | 0.14          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 1        | 0.14          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 14       | 0.14          |
| (1,737)  | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 17       | 0.14          |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 5        | 0.14          |
| (1,716)  | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 5        | 0.14          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 5        | 0.14          |
| (1,716)  | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 5        | 0.14          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 5        | 0.14          |
| (1,716)  | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 5        | 0.14          |
| (1,529)  | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 7        | 0.14          |
| (1,465)  | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 9        | 0.14          |
| (1,465)  | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 14       | 0.14          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 15       | 0.14          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 15       | 0.14          |
| (1,453)  | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 15       | 0.14          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 15       | 0.14          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 15       | 0.14          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 15       | 0.14          |
| (1,437) | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 11       | 0.14          |
| (1,437) | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 17       | 0.14          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 7        | 0.14          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 7        | 0.14          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 7        | 0.14          |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE1  | 11       | 0.14          |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE2  | 11       | 0.14          |
| (1,298) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE1  | 11       | 0.14          |
| (1,298) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE2  | 11       | 0.14          |
| (1,298) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE1  | 11       | 0.14          |
| (1,298) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE2  | 11       | 0.14          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 17       | 0.14          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 1        | 0.14          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 2        | 0.14          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 6        | 0.14          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 11       | 0.14          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 17       | 0.14          |
| (1,210) | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 7        | 0.14          |
| (1,210) | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 7        | 0.14          |
| (1,210) | 1:109:A:TYR:HA   | 1:219:B:PHE:HE1  | 10       | 0.14          |
| (1,210) | 1:109:A:TYR:HA   | 1:219:B:PHE:HE2  | 10       | 0.14          |
| (1,179) | 1:109:A:TYR:HE1  | 1:216:B:LYS:H    | 17       | 0.14          |
| (1,179) | 1:109:A:TYR:HE2  | 1:216:B:LYS:H    | 17       | 0.14          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 1        | 0.14          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 1        | 0.14          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 1        | 0.14          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 4        | 0.14          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 4        | 0.14          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 4        | 0.14          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 6        | 0.14          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 6        | 0.14          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 6        | 0.14          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 7        | 0.14          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 7        | 0.14          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 7        | 0.14          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 9        | 0.14          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 9        | 0.14          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 9        | 0.14          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 10       | 0.14          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,139)  | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 10       | 0.14          |
| (1,139)  | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 10       | 0.14          |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 4        | 0.14          |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 4        | 0.14          |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 4        | 0.14          |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 5        | 0.14          |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 5        | 0.14          |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 5        | 0.14          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 9        | 0.14          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 14       | 0.14          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 18       | 0.14          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 20       | 0.14          |
| (1,56)   | 1:106:A:ASP:HB3  | 1:214:B:ARG:HE   | 1        | 0.14          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 5        | 0.13          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 13       | 0.13          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 15       | 0.13          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 5        | 0.13          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 7        | 0.13          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 8        | 0.13          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 13       | 0.13          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 14       | 0.13          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 20       | 0.13          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 8        | 0.13          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 8        | 0.13          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 10       | 0.13          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 10       | 0.13          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 6        | 0.13          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 6        | 0.13          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 10       | 0.13          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 10       | 0.13          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 12       | 0.13          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 12       | 0.13          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 11       | 0.13          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 20       | 0.13          |
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H    | 11       | 0.13          |
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H    | 12       | 0.13          |
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H    | 18       | 0.13          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 19       | 0.13          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 19       | 0.13          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 19       | 0.13          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 19       | 0.13          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 19       | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 19       | 0.13          |
| (1,1139) | 1:136:A:GLN:HG2  | 1:139:A:VAL:HB   | 15       | 0.13          |
| (1,1139) | 1:136:A:GLN:HG3  | 1:139:A:VAL:HB   | 15       | 0.13          |
| (1,1110) | 1:135:A:VAL:HG11 | 1:339:C:VAL:H    | 5        | 0.13          |
| (1,1110) | 1:135:A:VAL:HG12 | 1:339:C:VAL:H    | 5        | 0.13          |
| (1,1110) | 1:135:A:VAL:HG13 | 1:339:C:VAL:H    | 5        | 0.13          |
| (1,1103) | 1:135:A:VAL:HG11 | 1:136:A:GLN:HA   | 16       | 0.13          |
| (1,1103) | 1:135:A:VAL:HG12 | 1:136:A:GLN:HA   | 16       | 0.13          |
| (1,1103) | 1:135:A:VAL:HG13 | 1:136:A:GLN:HA   | 16       | 0.13          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 15       | 0.13          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 15       | 0.13          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 17       | 0.13          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 17       | 0.13          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 13       | 0.13          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 13       | 0.13          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 16       | 0.13          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 16       | 0.13          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 11       | 0.13          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 11       | 0.13          |
| (1,1080) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HA   | 13       | 0.13          |
| (1,1080) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HA   | 13       | 0.13          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 15       | 0.13          |
| (1,1003) | 1:131:A:LEU:HA   | 1:343:C:CYS:HA   | 14       | 0.13          |
| (1,994)  | 1:131:A:LEU:HD11 | 1:335:C:VAL:H    | 16       | 0.13          |
| (1,994)  | 1:131:A:LEU:HD12 | 1:335:C:VAL:H    | 16       | 0.13          |
| (1,994)  | 1:131:A:LEU:HD13 | 1:335:C:VAL:H    | 16       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 1        | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 1        | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 2        | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 2        | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 11       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 11       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 13       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 13       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 14       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 14       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 16       | 0.13          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 16       | 0.13          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 5        | 0.13          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 13       | 0.13          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 15       | 0.13          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 3        | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 3        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 3        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 3        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 3        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 3        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 4        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 4        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 4        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 4        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 4        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 4        | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 10       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 10       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 10       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 10       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 10       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 10       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 14       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 14       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 14       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 14       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 14       | 0.13          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 14       | 0.13          |
| (1,801) | 1:125:A:TYR:HE1  | 1:126:A:LYS:HA   | 10       | 0.13          |
| (1,801) | 1:125:A:TYR:HE2  | 1:126:A:LYS:HA   | 10       | 0.13          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD11 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD12 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD13 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD11 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD12 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD13 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD11 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD12 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD13 | 2        | 0.13          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD11 | 13       | 0.13          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD12 | 13       | 0.13          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD13 | 13       | 0.13          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD11 | 13       | 0.13          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD12 | 13       | 0.13          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD13 | 13       | 0.13          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD11 | 13       | 0.13          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD12 | 13       | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD13 | 13       | 0.13          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 4        | 0.13          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 4        | 0.13          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 4        | 0.13          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 4        | 0.13          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 4        | 0.13          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 4        | 0.13          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 6        | 0.13          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 6        | 0.13          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 6        | 0.13          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 6        | 0.13          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 6        | 0.13          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 6        | 0.13          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 4        | 0.13          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 4        | 0.13          |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE2  | 7        | 0.13          |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE3  | 7        | 0.13          |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE2  | 7        | 0.13          |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE3  | 7        | 0.13          |
| (1,529) | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 14       | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 9        | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 9        | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 9        | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 9        | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 9        | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 9        | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 14       | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 14       | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 14       | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 14       | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 14       | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 14       | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 19       | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 19       | 0.13          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 19       | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 19       | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 19       | 0.13          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 19       | 0.13          |
| (1,437) | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 8        | 0.13          |
| (1,437) | 1:114:A:ARG:H    | 1:449:D:ILE:HA   | 18       | 0.13          |
| (1,404) | 1:113:A:ILE:HD11 | 1:226:B:LYS:HA   | 17       | 0.13          |
| (1,404) | 1:113:A:ILE:HD12 | 1:226:B:LYS:HA   | 17       | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,404) | 1:113:A:ILE:HD13 | 1:226:B:LYS:HA   | 17       | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 1        | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 1        | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 1        | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 6        | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 6        | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 6        | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 15       | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 15       | 0.13          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 15       | 0.13          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 5        | 0.13          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 5        | 0.13          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 5        | 0.13          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 10       | 0.13          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 10       | 0.13          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 10       | 0.13          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 19       | 0.13          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 19       | 0.13          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 19       | 0.13          |
| (1,315) | 1:111:A:LEU:HD21 | 1:226:B:LYS:HA   | 4        | 0.13          |
| (1,315) | 1:111:A:LEU:HD22 | 1:226:B:LYS:HA   | 4        | 0.13          |
| (1,315) | 1:111:A:LEU:HD23 | 1:226:B:LYS:HA   | 4        | 0.13          |
| (1,315) | 1:111:A:LEU:HD21 | 1:226:B:LYS:HA   | 13       | 0.13          |
| (1,315) | 1:111:A:LEU:HD22 | 1:226:B:LYS:HA   | 13       | 0.13          |
| (1,315) | 1:111:A:LEU:HD23 | 1:226:B:LYS:HA   | 13       | 0.13          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 9        | 0.13          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 10       | 0.13          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 11       | 0.13          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 13       | 0.13          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 18       | 0.13          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 20       | 0.13          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 5        | 0.13          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 5        | 0.13          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 5        | 0.13          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 8        | 0.13          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 8        | 0.13          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 8        | 0.13          |
| (1,121) | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 7        | 0.13          |
| (1,121) | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 7        | 0.13          |
| (1,121) | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 7        | 0.13          |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE1  | 15       | 0.13          |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE2  | 15       | 0.13          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 6        | 0.13          |
| (1,56)   | 1:106:A:ASP:HB3  | 1:214:B:ARG:HE   | 20       | 0.13          |
| (1,19)   | 1:104:A:ASP:HB2  | 1:218:B:LYS:H    | 4        | 0.13          |
| (1,19)   | 1:104:A:ASP:HB3  | 1:218:B:LYS:H    | 4        | 0.13          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 14       | 0.12          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 4        | 0.12          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 18       | 0.12          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 19       | 0.12          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 5        | 0.12          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 5        | 0.12          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 6        | 0.12          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 6        | 0.12          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 11       | 0.12          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 11       | 0.12          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 19       | 0.12          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 19       | 0.12          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 9        | 0.12          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 9        | 0.12          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 13       | 0.12          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 13       | 0.12          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 15       | 0.12          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 15       | 0.12          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 2        | 0.12          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 10       | 0.12          |
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H    | 13       | 0.12          |
| (1,1298) | 1:143:A:CYS:HB2  | 1:144:A:CYS:HA   | 1        | 0.12          |
| (1,1291) | 1:142:A:ALA:HB1  | 1:146:A:ARG:H    | 9        | 0.12          |
| (1,1291) | 1:142:A:ALA:HB2  | 1:146:A:ARG:H    | 9        | 0.12          |
| (1,1291) | 1:142:A:ALA:HB3  | 1:146:A:ARG:H    | 9        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 6        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 6        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 6        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 6        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 6        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 6        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 8        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 8        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 8        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 8        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 8        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 8        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE2  | 9        | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1220) | 1:139:A:VAL:HG21 | 1:140:A:LYS:HE3  | 9        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE2  | 9        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG22 | 1:140:A:LYS:HE3  | 9        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE2  | 9        | 0.12          |
| (1,1220) | 1:139:A:VAL:HG23 | 1:140:A:LYS:HE3  | 9        | 0.12          |
| (1,1103) | 1:135:A:VAL:HG11 | 1:136:A:GLN:HA   | 5        | 0.12          |
| (1,1103) | 1:135:A:VAL:HG12 | 1:136:A:GLN:HA   | 5        | 0.12          |
| (1,1103) | 1:135:A:VAL:HG13 | 1:136:A:GLN:HA   | 5        | 0.12          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 3        | 0.12          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 3        | 0.12          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2  | 18       | 0.12          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2  | 18       | 0.12          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3  | 7        | 0.12          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3  | 7        | 0.12          |
| (1,1055) | 1:134:A:TYR:H    | 1:140:A:LYS:HD2  | 11       | 0.12          |
| (1,1055) | 1:134:A:TYR:H    | 1:140:A:LYS:HD3  | 11       | 0.12          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 8        | 0.12          |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 14       | 0.12          |
| (1,1003) | 1:131:A:LEU:HA   | 1:343:C:CYS:HA   | 8        | 0.12          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1  | 15       | 0.12          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2  | 15       | 0.12          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 6        | 0.12          |
| (1,903)  | 1:128:A:ALA:HB1  | 1:330:C:ASP:H    | 11       | 0.12          |
| (1,903)  | 1:128:A:ALA:HB2  | 1:330:C:ASP:H    | 11       | 0.12          |
| (1,903)  | 1:128:A:ALA:HB3  | 1:330:C:ASP:H    | 11       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 10       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 10       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 10       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 11       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 11       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 11       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 18       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 18       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 18       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 19       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 19       | 0.12          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 19       | 0.12          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 1        | 0.12          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 1        | 0.12          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 1        | 0.12          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 1        | 0.12          |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 1        | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 1        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 2        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 2        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 2        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 2        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 2        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 2        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 9        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 9        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 9        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 9        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 9        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 9        | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 20       | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 20       | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 20       | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 20       | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 20       | 0.12          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 20       | 0.12          |
| (1,743) | 1:123:A:LYS:H    | 1:123:A:LYS:HE2  | 4        | 0.12          |
| (1,743) | 1:123:A:LYS:H    | 1:123:A:LYS:HE3  | 4        | 0.12          |
| (1,737) | 1:123:A:LYS:HA   | 1:123:A:LYS:HD2  | 8        | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 9        | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 9        | 0.12          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 9        | 0.12          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 9        | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 9        | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 9        | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 10       | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 10       | 0.12          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 10       | 0.12          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 10       | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 10       | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 10       | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 13       | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 13       | 0.12          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 13       | 0.12          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 13       | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 13       | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 13       | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 16       | 0.12          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 16       | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 16       | 0.12          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 16       | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 16       | 0.12          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 16       | 0.12          |
| (1,676) | 1:121:A:LYS:HA   | 1:229:B:LEU:HD11 | 1        | 0.12          |
| (1,676) | 1:121:A:LYS:HA   | 1:229:B:LEU:HD12 | 1        | 0.12          |
| (1,676) | 1:121:A:LYS:HA   | 1:229:B:LEU:HD13 | 1        | 0.12          |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD11 | 4        | 0.12          |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD12 | 4        | 0.12          |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD13 | 4        | 0.12          |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD11 | 5        | 0.12          |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD12 | 5        | 0.12          |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD13 | 5        | 0.12          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 5        | 0.12          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 5        | 0.12          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 6        | 0.12          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 6        | 0.12          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 13       | 0.12          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 13       | 0.12          |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE2  | 10       | 0.12          |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE3  | 10       | 0.12          |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE2  | 10       | 0.12          |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE3  | 10       | 0.12          |
| (1,610) | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE2  | 6        | 0.12          |
| (1,610) | 1:119:A:PHE:HZ   | 1:123:A:LYS:HE3  | 6        | 0.12          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG21 | 2        | 0.12          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG22 | 2        | 0.12          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG23 | 2        | 0.12          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG21 | 2        | 0.12          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG22 | 2        | 0.12          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG23 | 2        | 0.12          |
| (1,562) | 1:118:A:LYS:HE3  | 1:229:B:LEU:HB3  | 14       | 0.12          |
| (1,533) | 1:118:A:LYS:H    | 1:118:A:LYS:HE3  | 14       | 0.12          |
| (1,529) | 1:118:A:LYS:H    | 1:118:A:LYS:HD3  | 3        | 0.12          |
| (1,465) | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 19       | 0.12          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 6        | 0.12          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 6        | 0.12          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 6        | 0.12          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 6        | 0.12          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 6        | 0.12          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 6        | 0.12          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG21 | 7        | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG22 | 7        | 0.12          |
| (1,453) | 1:114:A:ARG:HD2  | 1:449:D:ILE:HG23 | 7        | 0.12          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG21 | 7        | 0.12          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG22 | 7        | 0.12          |
| (1,453) | 1:114:A:ARG:HD3  | 1:449:D:ILE:HG23 | 7        | 0.12          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 3        | 0.12          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 3        | 0.12          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 3        | 0.12          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 15       | 0.12          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 15       | 0.12          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 15       | 0.12          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 16       | 0.12          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 16       | 0.12          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 16       | 0.12          |
| (1,315) | 1:111:A:LEU:HD21 | 1:226:B:LYS:HA   | 18       | 0.12          |
| (1,315) | 1:111:A:LEU:HD22 | 1:226:B:LYS:HA   | 18       | 0.12          |
| (1,315) | 1:111:A:LEU:HD23 | 1:226:B:LYS:HA   | 18       | 0.12          |
| (1,281) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HA   | 7        | 0.12          |
| (1,281) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HA   | 7        | 0.12          |
| (1,281) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HA   | 7        | 0.12          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 6        | 0.12          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 7        | 0.12          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 12       | 0.12          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 14       | 0.12          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 19       | 0.12          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 20       | 0.12          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 9        | 0.12          |
| (1,224) | 1:110:A:THR:HG21 | 1:112:A:ASN:HA   | 8        | 0.12          |
| (1,224) | 1:110:A:THR:HG22 | 1:112:A:ASN:HA   | 8        | 0.12          |
| (1,224) | 1:110:A:THR:HG23 | 1:112:A:ASN:HA   | 8        | 0.12          |
| (1,224) | 1:110:A:THR:HG21 | 1:112:A:ASN:HA   | 16       | 0.12          |
| (1,224) | 1:110:A:THR:HG22 | 1:112:A:ASN:HA   | 16       | 0.12          |
| (1,224) | 1:110:A:THR:HG23 | 1:112:A:ASN:HA   | 16       | 0.12          |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 16       | 0.12          |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 16       | 0.12          |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 16       | 0.12          |
| (1,122) | 1:108:A:VAL:HG11 | 1:212:B:ASN:HA   | 3        | 0.12          |
| (1,122) | 1:108:A:VAL:HG12 | 1:212:B:ASN:HA   | 3        | 0.12          |
| (1,122) | 1:108:A:VAL:HG13 | 1:212:B:ASN:HA   | 3        | 0.12          |
| (1,122) | 1:108:A:VAL:HG11 | 1:212:B:ASN:HA   | 5        | 0.12          |
| (1,122) | 1:108:A:VAL:HG12 | 1:212:B:ASN:HA   | 5        | 0.12          |
| (1,122) | 1:108:A:VAL:HG13 | 1:212:B:ASN:HA   | 5        | 0.12          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,122)  | 1:108:A:VAL:HG11 | 1:212:B:ASN:HA   | 7        | 0.12          |
| (1,122)  | 1:108:A:VAL:HG12 | 1:212:B:ASN:HA   | 7        | 0.12          |
| (1,122)  | 1:108:A:VAL:HG13 | 1:212:B:ASN:HA   | 7        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 1        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 1        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 1        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 3        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 3        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 3        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 6        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 6        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 6        | 0.12          |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 13       | 0.12          |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 13       | 0.12          |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 13       | 0.12          |
| (1,121)  | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 19       | 0.12          |
| (1,121)  | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 19       | 0.12          |
| (1,121)  | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 19       | 0.12          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 8        | 0.12          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 11       | 0.12          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 12       | 0.12          |
| (1,64)   | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 13       | 0.12          |
| (3,33)   | 1:141:A:LYS:O    | 1:145:A:GLN:H    | 19       | 0.11          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 2        | 0.11          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 6        | 0.11          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 9        | 0.11          |
| (3,1)    | 1:117:A:ARG:O    | 1:121:A:LYS:H    | 11       | 0.11          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 3        | 0.11          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 3        | 0.11          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 17       | 0.11          |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 17       | 0.11          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 4        | 0.11          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 4        | 0.11          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB2  | 5        | 0.11          |
| (1,1353) | 1:146:A:ARG:H    | 1:147:A:ASN:HB3  | 5        | 0.11          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 8        | 0.11          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 9        | 0.11          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 17       | 0.11          |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 18       | 0.11          |
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD2  | 6        | 0.11          |
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3  | 6        | 0.11          |
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD2  | 12       | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1342) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3 | 12       | 0.11          |
| (1,1334) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3 | 6        | 0.11          |
| (1,1334) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3 | 12       | 0.11          |
| (1,1334) | 1:146:A:ARG:HA   | 1:146:A:ARG:HD3 | 17       | 0.11          |
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H   | 10       | 0.11          |
| (1,1332) | 1:145:A:GLN:HA   | 1:148:A:GLN:H   | 20       | 0.11          |
| (1,1298) | 1:143:A:CYS:HB2  | 1:144:A:CYS:HA  | 8        | 0.11          |
| (1,1298) | 1:143:A:CYS:HB2  | 1:144:A:CYS:HA  | 10       | 0.11          |
| (1,1298) | 1:143:A:CYS:HB2  | 1:144:A:CYS:HA  | 12       | 0.11          |
| (1,1291) | 1:142:A:ALA:HB1  | 1:146:A:ARG:H   | 20       | 0.11          |
| (1,1291) | 1:142:A:ALA:HB2  | 1:146:A:ARG:H   | 20       | 0.11          |
| (1,1291) | 1:142:A:ALA:HB3  | 1:146:A:ARG:H   | 20       | 0.11          |
| (1,1272) | 1:141:A:LYS:HE2  | 1:142:A:ALA:H   | 20       | 0.11          |
| (1,1272) | 1:141:A:LYS:HE3  | 1:142:A:ALA:H   | 20       | 0.11          |
| (1,1139) | 1:136:A:GLN:HG2  | 1:139:A:VAL:HB  | 3        | 0.11          |
| (1,1139) | 1:136:A:GLN:HG3  | 1:139:A:VAL:HB  | 3        | 0.11          |
| (1,1139) | 1:136:A:GLN:HG2  | 1:139:A:VAL:HB  | 9        | 0.11          |
| (1,1139) | 1:136:A:GLN:HG3  | 1:139:A:VAL:HB  | 9        | 0.11          |
| (1,1139) | 1:136:A:GLN:HG2  | 1:139:A:VAL:HB  | 16       | 0.11          |
| (1,1139) | 1:136:A:GLN:HG3  | 1:139:A:VAL:HB  | 16       | 0.11          |
| (1,1103) | 1:135:A:VAL:HG11 | 1:136:A:GLN:HA  | 11       | 0.11          |
| (1,1103) | 1:135:A:VAL:HG12 | 1:136:A:GLN:HA  | 11       | 0.11          |
| (1,1103) | 1:135:A:VAL:HG13 | 1:136:A:GLN:HA  | 11       | 0.11          |
| (1,1103) | 1:135:A:VAL:HG11 | 1:136:A:GLN:HA  | 15       | 0.11          |
| (1,1103) | 1:135:A:VAL:HG12 | 1:136:A:GLN:HA  | 15       | 0.11          |
| (1,1103) | 1:135:A:VAL:HG13 | 1:136:A:GLN:HA  | 15       | 0.11          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2 | 1        | 0.11          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2 | 1        | 0.11          |
| (1,1086) | 1:134:A:TYR:HD1  | 1:346:C:ARG:HG2 | 12       | 0.11          |
| (1,1086) | 1:134:A:TYR:HD2  | 1:346:C:ARG:HG2 | 12       | 0.11          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3 | 1        | 0.11          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3 | 1        | 0.11          |
| (1,1085) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HD3 | 18       | 0.11          |
| (1,1085) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HD3 | 18       | 0.11          |
| (1,1079) | 1:134:A:TYR:HE1  | 1:346:C:ARG:HA  | 6        | 0.11          |
| (1,1079) | 1:134:A:TYR:HE2  | 1:346:C:ARG:HA  | 6        | 0.11          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE1 | 5        | 0.11          |
| (1,981)  | 1:131:A:LEU:HA   | 1:134:A:TYR:HE2 | 5        | 0.11          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG  | 7        | 0.11          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG  | 10       | 0.11          |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG  | 18       | 0.11          |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1 | 2        | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,896) | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 2        | 0.11          |
| (1,896) | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 2        | 0.11          |
| (1,896) | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 3        | 0.11          |
| (1,896) | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 3        | 0.11          |
| (1,896) | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 3        | 0.11          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 16       | 0.11          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 16       | 0.11          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 16       | 0.11          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 16       | 0.11          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 16       | 0.11          |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 16       | 0.11          |
| (1,815) | 1:125:A:TYR:HE1  | 1:132:A:LEU:HG   | 6        | 0.11          |
| (1,815) | 1:125:A:TYR:HE2  | 1:132:A:LEU:HG   | 6        | 0.11          |
| (1,815) | 1:125:A:TYR:HE1  | 1:132:A:LEU:HG   | 9        | 0.11          |
| (1,815) | 1:125:A:TYR:HE2  | 1:132:A:LEU:HG   | 9        | 0.11          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD11 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD12 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG11 | 1:229:B:LEU:HD13 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD11 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD12 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG12 | 1:229:B:LEU:HD13 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD11 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD12 | 14       | 0.11          |
| (1,728) | 1:122:A:VAL:HG13 | 1:229:B:LEU:HD13 | 14       | 0.11          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 3        | 0.11          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 3        | 0.11          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 3        | 0.11          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 3        | 0.11          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 3        | 0.11          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 3        | 0.11          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 18       | 0.11          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 18       | 0.11          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 18       | 0.11          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 18       | 0.11          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 18       | 0.11          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 18       | 0.11          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 20       | 0.11          |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 20       | 0.11          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 20       | 0.11          |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 20       | 0.11          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 20       | 0.11          |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 20       | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 1        | 0.11          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 1        | 0.11          |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 19       | 0.11          |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 19       | 0.11          |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE2  | 2        | 0.11          |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE3  | 2        | 0.11          |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE2  | 2        | 0.11          |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE3  | 2        | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG21 | 10       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG22 | 10       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG23 | 10       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG21 | 10       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG22 | 10       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG23 | 10       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG21 | 14       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG22 | 14       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG23 | 14       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG21 | 14       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG22 | 14       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG23 | 14       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG21 | 18       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG22 | 18       | 0.11          |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG23 | 18       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG21 | 18       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG22 | 18       | 0.11          |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG23 | 18       | 0.11          |
| (1,532) | 1:118:A:LYS:H    | 1:118:A:LYS:HE2  | 5        | 0.11          |
| (1,525) | 1:117:A:ARG:H    | 1:121:A:LYS:HE3  | 12       | 0.11          |
| (1,465) | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 1        | 0.11          |
| (1,465) | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 6        | 0.11          |
| (1,465) | 1:116:A:LYS:HA   | 1:116:A:LYS:HD2  | 7        | 0.11          |
| (1,421) | 1:114:A:ARG:H    | 1:114:A:ARG:HD2  | 8        | 0.11          |
| (1,404) | 1:113:A:ILE:HD11 | 1:226:B:LYS:HA   | 4        | 0.11          |
| (1,404) | 1:113:A:ILE:HD12 | 1:226:B:LYS:HA   | 4        | 0.11          |
| (1,404) | 1:113:A:ILE:HD13 | 1:226:B:LYS:HA   | 4        | 0.11          |
| (1,404) | 1:113:A:ILE:HD11 | 1:226:B:LYS:HA   | 7        | 0.11          |
| (1,404) | 1:113:A:ILE:HD12 | 1:226:B:LYS:HA   | 7        | 0.11          |
| (1,404) | 1:113:A:ILE:HD13 | 1:226:B:LYS:HA   | 7        | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 11       | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 11       | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 11       | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 16       | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 16       | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 16       | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 18       | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 18       | 0.11          |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 18       | 0.11          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 9        | 0.11          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 9        | 0.11          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 9        | 0.11          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 18       | 0.11          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 18       | 0.11          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 18       | 0.11          |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 20       | 0.11          |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 20       | 0.11          |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 20       | 0.11          |
| (1,278) | 1:111:A:LEU:H    | 1:213:B:ILE:HD11 | 10       | 0.11          |
| (1,278) | 1:111:A:LEU:H    | 1:213:B:ILE:HD12 | 10       | 0.11          |
| (1,278) | 1:111:A:LEU:H    | 1:213:B:ILE:HD13 | 10       | 0.11          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 1        | 0.11          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 3        | 0.11          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 5        | 0.11          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 8        | 0.11          |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 16       | 0.11          |
| (1,228) | 1:110:A:THR:HA   | 1:211:B:LEU:H    | 19       | 0.11          |
| (1,224) | 1:110:A:THR:HG21 | 1:112:A:ASN:HA   | 1        | 0.11          |
| (1,224) | 1:110:A:THR:HG22 | 1:112:A:ASN:HA   | 1        | 0.11          |
| (1,224) | 1:110:A:THR:HG23 | 1:112:A:ASN:HA   | 1        | 0.11          |
| (1,224) | 1:110:A:THR:HG21 | 1:112:A:ASN:HA   | 9        | 0.11          |
| (1,224) | 1:110:A:THR:HG22 | 1:112:A:ASN:HA   | 9        | 0.11          |
| (1,224) | 1:110:A:THR:HG23 | 1:112:A:ASN:HA   | 9        | 0.11          |
| (1,121) | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 11       | 0.11          |
| (1,121) | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 11       | 0.11          |
| (1,121) | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 11       | 0.11          |
| (1,121) | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 14       | 0.11          |
| (1,121) | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 14       | 0.11          |
| (1,121) | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 14       | 0.11          |
| (1,121) | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA   | 20       | 0.11          |
| (1,121) | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA   | 20       | 0.11          |
| (1,121) | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA   | 20       | 0.11          |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE1  | 7        | 0.11          |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE2  | 7        | 0.11          |
| (1,64)  | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 10       | 0.11          |
| (1,64)  | 1:106:A:ASP:HB2  | 1:215:B:GLY:H    | 15       | 0.11          |

*Continued on next page...*

*Continued from previous page...*

| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,49)   | 1:106:A:ASP:H    | 1:107:A:VAL:HG11 | 9        | 0.11          |
| (1,49)   | 1:106:A:ASP:H    | 1:107:A:VAL:HG12 | 9        | 0.11          |
| (1,49)   | 1:106:A:ASP:H    | 1:107:A:VAL:HG13 | 9        | 0.11          |
| (1,33)   | 1:105:A:GLY:HA2  | 1:216:B:LYS:H    | 12       | 0.11          |
| (1,33)   | 1:105:A:GLY:HA3  | 1:216:B:LYS:H    | 12       | 0.11          |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 2        | 0.1           |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 2        | 0.1           |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 7        | 0.1           |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 7        | 0.1           |
| (1,1383) | 1:148:A:GLN:HB2  | 1:149:A:ILE:HG13 | 16       | 0.1           |
| (1,1383) | 1:148:A:GLN:HB3  | 1:149:A:ILE:HG13 | 16       | 0.1           |
| (1,1351) | 1:146:A:ARG:HD2  | 1:147:A:ASN:H    | 13       | 0.1           |
| (1,1298) | 1:143:A:CYS:HB2  | 1:144:A:CYS:HA   | 20       | 0.1           |
| (1,1202) | 1:138:A:ASP:HB2  | 1:142:A:ALA:HB1  | 9        | 0.1           |
| (1,1202) | 1:138:A:ASP:HB2  | 1:142:A:ALA:HB2  | 9        | 0.1           |
| (1,1202) | 1:138:A:ASP:HB2  | 1:142:A:ALA:HB3  | 9        | 0.1           |
| (1,1152) | 1:137:A:PRO:HB3  | 1:138:A:ASP:HA   | 16       | 0.1           |
| (1,1103) | 1:135:A:VAL:HG11 | 1:136:A:GLN:HA   | 7        | 0.1           |
| (1,1103) | 1:135:A:VAL:HG12 | 1:136:A:GLN:HA   | 7        | 0.1           |
| (1,1103) | 1:135:A:VAL:HG13 | 1:136:A:GLN:HA   | 7        | 0.1           |
| (1,1051) | 1:134:A:TYR:HD1  | 1:135:A:VAL:HG21 | 18       | 0.1           |
| (1,1051) | 1:134:A:TYR:HD1  | 1:135:A:VAL:HG22 | 18       | 0.1           |
| (1,1051) | 1:134:A:TYR:HD1  | 1:135:A:VAL:HG23 | 18       | 0.1           |
| (1,1051) | 1:134:A:TYR:HD2  | 1:135:A:VAL:HG21 | 18       | 0.1           |
| (1,1051) | 1:134:A:TYR:HD2  | 1:135:A:VAL:HG22 | 18       | 0.1           |
| (1,1051) | 1:134:A:TYR:HD2  | 1:135:A:VAL:HG23 | 18       | 0.1           |
| (1,1047) | 1:134:A:TYR:H    | 1:135:A:VAL:HB   | 7        | 0.1           |
| (1,908)  | 1:128:A:ALA:H    | 1:332:C:LEU:HG   | 4        | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 8        | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 8        | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 8        | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 9        | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 9        | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 9        | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 13       | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 13       | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 13       | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB1  | 17       | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB2  | 17       | 0.1           |
| (1,896)  | 1:128:A:ALA:H    | 1:328:C:ALA:HB3  | 17       | 0.1           |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD11 | 13       | 0.1           |
| (1,884)  | 1:127:A:GLU:H    | 1:332:C:LEU:HD12 | 13       | 0.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD13 | 13       | 0.1           |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD21 | 13       | 0.1           |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD22 | 13       | 0.1           |
| (1,884) | 1:127:A:GLU:H    | 1:332:C:LEU:HD23 | 13       | 0.1           |
| (1,815) | 1:125:A:TYR:HE1  | 1:132:A:LEU:HG   | 11       | 0.1           |
| (1,815) | 1:125:A:TYR:HE2  | 1:132:A:LEU:HG   | 11       | 0.1           |
| (1,815) | 1:125:A:TYR:HE1  | 1:132:A:LEU:HG   | 19       | 0.1           |
| (1,815) | 1:125:A:TYR:HE2  | 1:132:A:LEU:HG   | 19       | 0.1           |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE1  | 1        | 0.1           |
| (1,716) | 1:122:A:VAL:HG21 | 1:225:B:TYR:HE2  | 1        | 0.1           |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE1  | 1        | 0.1           |
| (1,716) | 1:122:A:VAL:HG22 | 1:225:B:TYR:HE2  | 1        | 0.1           |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE1  | 1        | 0.1           |
| (1,716) | 1:122:A:VAL:HG23 | 1:225:B:TYR:HE2  | 1        | 0.1           |
| (1,676) | 1:121:A:LYS:HA   | 1:229:B:LEU:HD11 | 13       | 0.1           |
| (1,676) | 1:121:A:LYS:HA   | 1:229:B:LEU:HD12 | 13       | 0.1           |
| (1,676) | 1:121:A:LYS:HA   | 1:229:B:LEU:HD13 | 13       | 0.1           |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD11 | 2        | 0.1           |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD12 | 2        | 0.1           |
| (1,675) | 1:121:A:LYS:H    | 1:229:B:LEU:HD13 | 2        | 0.1           |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 3        | 0.1           |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 3        | 0.1           |
| (1,657) | 1:121:A:LYS:HE2  | 1:122:A:VAL:H    | 7        | 0.1           |
| (1,657) | 1:121:A:LYS:HE3  | 1:122:A:VAL:H    | 7        | 0.1           |
| (1,627) | 1:120:A:GLU:HA   | 1:123:A:LYS:HB2  | 3        | 0.1           |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE2  | 4        | 0.1           |
| (1,611) | 1:119:A:PHE:HD1  | 1:123:A:LYS:HE3  | 4        | 0.1           |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE2  | 4        | 0.1           |
| (1,611) | 1:119:A:PHE:HD2  | 1:123:A:LYS:HE3  | 4        | 0.1           |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG21 | 17       | 0.1           |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG22 | 17       | 0.1           |
| (1,594) | 1:119:A:PHE:HE1  | 1:122:A:VAL:HG23 | 17       | 0.1           |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG21 | 17       | 0.1           |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG22 | 17       | 0.1           |
| (1,594) | 1:119:A:PHE:HE2  | 1:122:A:VAL:HG23 | 17       | 0.1           |
| (1,517) | 1:117:A:ARG:H    | 1:118:A:LYS:HE2  | 4        | 0.1           |
| (1,517) | 1:117:A:ARG:H    | 1:118:A:LYS:HE3  | 4        | 0.1           |
| (1,517) | 1:117:A:ARG:H    | 1:118:A:LYS:HE2  | 11       | 0.1           |
| (1,517) | 1:117:A:ARG:H    | 1:118:A:LYS:HE3  | 11       | 0.1           |
| (1,466) | 1:116:A:LYS:H    | 1:116:A:LYS:HD2  | 5        | 0.1           |
| (1,404) | 1:113:A:ILE:HD11 | 1:226:B:LYS:HA   | 14       | 0.1           |
| (1,404) | 1:113:A:ILE:HD12 | 1:226:B:LYS:HA   | 14       | 0.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|---------|------------------|------------------|----------|---------------|
| (1,404) | 1:113:A:ILE:HD13 | 1:226:B:LYS:HA   | 14       | 0.1           |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG21 | 13       | 0.1           |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG22 | 13       | 0.1           |
| (1,354) | 1:112:A:ASN:H    | 1:449:D:ILE:HG23 | 13       | 0.1           |
| (1,337) | 1:112:A:ASN:HB2  | 1:449:D:ILE:H    | 3        | 0.1           |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 8        | 0.1           |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 8        | 0.1           |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 8        | 0.1           |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 12       | 0.1           |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 12       | 0.1           |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 12       | 0.1           |
| (1,321) | 1:111:A:LEU:HD21 | 1:227:B:GLU:H    | 14       | 0.1           |
| (1,321) | 1:111:A:LEU:HD22 | 1:227:B:GLU:H    | 14       | 0.1           |
| (1,321) | 1:111:A:LEU:HD23 | 1:227:B:GLU:H    | 14       | 0.1           |
| (1,315) | 1:111:A:LEU:HD21 | 1:226:B:LYS:HA   | 11       | 0.1           |
| (1,315) | 1:111:A:LEU:HD22 | 1:226:B:LYS:HA   | 11       | 0.1           |
| (1,315) | 1:111:A:LEU:HD23 | 1:226:B:LYS:HA   | 11       | 0.1           |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE1  | 3        | 0.1           |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE2  | 3        | 0.1           |
| (1,298) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE1  | 3        | 0.1           |
| (1,298) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE2  | 3        | 0.1           |
| (1,298) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE1  | 3        | 0.1           |
| (1,298) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE2  | 3        | 0.1           |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE1  | 18       | 0.1           |
| (1,298) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HE2  | 18       | 0.1           |
| (1,298) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE1  | 18       | 0.1           |
| (1,298) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HE2  | 18       | 0.1           |
| (1,298) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE1  | 18       | 0.1           |
| (1,298) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HE2  | 18       | 0.1           |
| (1,281) | 1:111:A:LEU:HD21 | 1:219:B:PHE:HA   | 15       | 0.1           |
| (1,281) | 1:111:A:LEU:HD22 | 1:219:B:PHE:HA   | 15       | 0.1           |
| (1,281) | 1:111:A:LEU:HD23 | 1:219:B:PHE:HA   | 15       | 0.1           |
| (1,278) | 1:111:A:LEU:H    | 1:213:B:ILE:HD11 | 14       | 0.1           |
| (1,278) | 1:111:A:LEU:H    | 1:213:B:ILE:HD12 | 14       | 0.1           |
| (1,278) | 1:111:A:LEU:H    | 1:213:B:ILE:HD13 | 14       | 0.1           |
| (1,232) | 1:110:A:THR:HB   | 1:212:B:ASN:HA   | 2        | 0.1           |
| (1,139) | 1:108:A:VAL:HG11 | 1:214:B:ARG:HE   | 11       | 0.1           |
| (1,139) | 1:108:A:VAL:HG12 | 1:214:B:ARG:HE   | 11       | 0.1           |
| (1,139) | 1:108:A:VAL:HG13 | 1:214:B:ARG:HE   | 11       | 0.1           |
| (1,122) | 1:108:A:VAL:HG11 | 1:212:B:ASN:HA   | 6        | 0.1           |
| (1,122) | 1:108:A:VAL:HG12 | 1:212:B:ASN:HA   | 6        | 0.1           |
| (1,122) | 1:108:A:VAL:HG13 | 1:212:B:ASN:HA   | 6        | 0.1           |

*Continued on next page...*

*Continued from previous page...*

| Key     | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|---------|------------------|-----------------|----------|---------------|
| (1,122) | 1:108:A:VAL:HG11 | 1:212:B:ASN:HA  | 15       | 0.1           |
| (1,122) | 1:108:A:VAL:HG12 | 1:212:B:ASN:HA  | 15       | 0.1           |
| (1,122) | 1:108:A:VAL:HG13 | 1:212:B:ASN:HA  | 15       | 0.1           |
| (1,122) | 1:108:A:VAL:HG11 | 1:212:B:ASN:HA  | 20       | 0.1           |
| (1,122) | 1:108:A:VAL:HG12 | 1:212:B:ASN:HA  | 20       | 0.1           |
| (1,122) | 1:108:A:VAL:HG13 | 1:212:B:ASN:HA  | 20       | 0.1           |
| (1,121) | 1:108:A:VAL:HG21 | 1:212:B:ASN:HA  | 10       | 0.1           |
| (1,121) | 1:108:A:VAL:HG22 | 1:212:B:ASN:HA  | 10       | 0.1           |
| (1,121) | 1:108:A:VAL:HG23 | 1:212:B:ASN:HA  | 10       | 0.1           |
| (1,102) | 1:107:A:VAL:HG11 | 1:216:B:LYS:H   | 7        | 0.1           |
| (1,102) | 1:107:A:VAL:HG12 | 1:216:B:LYS:H   | 7        | 0.1           |
| (1,102) | 1:107:A:VAL:HG13 | 1:216:B:LYS:H   | 7        | 0.1           |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE1 | 3        | 0.1           |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE2 | 3        | 0.1           |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE1 | 8        | 0.1           |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE2 | 8        | 0.1           |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE1 | 13       | 0.1           |
| (1,87)  | 1:107:A:VAL:H    | 1:109:A:TYR:HE2 | 13       | 0.1           |
| (1,64)  | 1:106:A:ASP:HB2  | 1:215:B:GLY:H   | 1        | 0.1           |
| (1,56)  | 1:106:A:ASP:HB3  | 1:214:B:ARG:HE  | 3        | 0.1           |

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

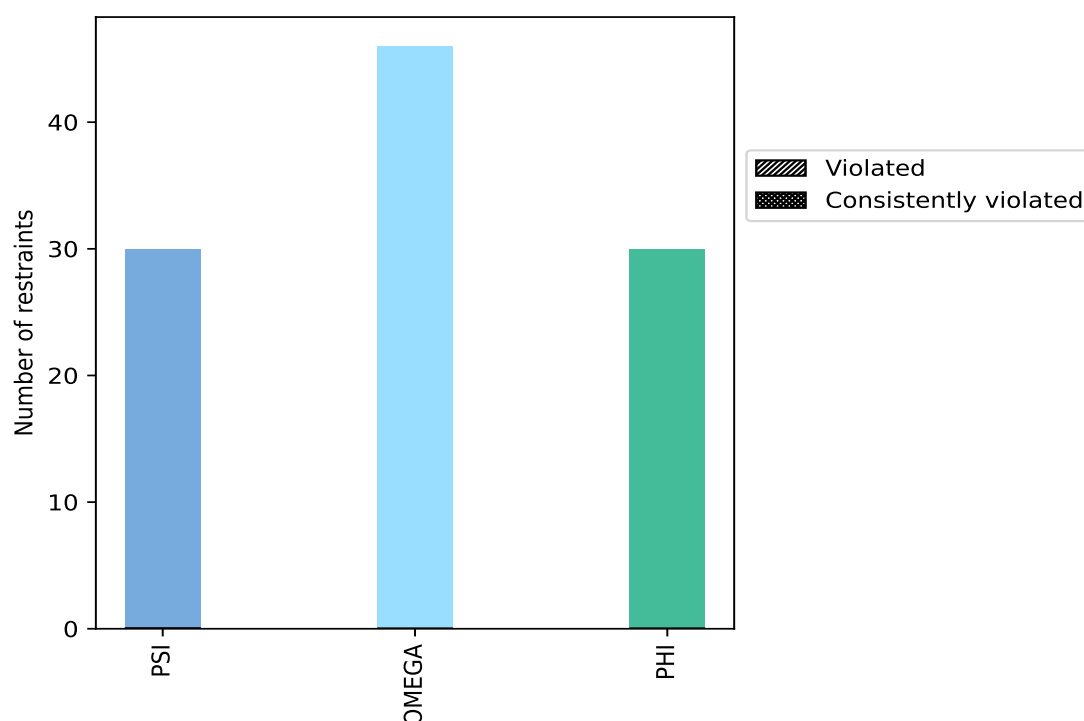
### 10.1 Summary of dihedral-angle violations [i](#)

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 | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 30    | 28.3           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| OMEGA      | 46    | 43.4           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| PHI        | 30    | 28.3           | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total      | 106   | 100.0          | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> 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](#)

No violations found

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

No violations found

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

No violations found

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

No violations found