



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 24, 2024 – 04:47 PM EST

PDB ID : 2LNQ  
BMRB ID : 18175  
Title : 40-residue D23N beta amyloid fibril  
Authors : Qiang, W.; Yau, W.; Luo, Y.; Mattson, M.P.; Tycko, R.  
Deposited on : 2012-01-03

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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

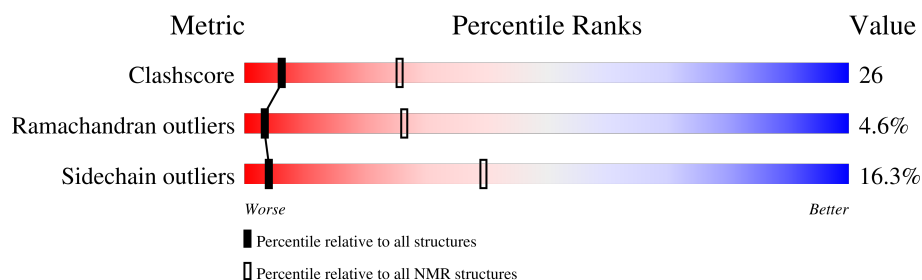
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 3%.

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            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 40     | 42% 10% 12% 35%   |
| 1   | B     | 40     | 32% 25% 8% 35%    |
| 1   | C     | 40     | 35% 18% 5% 8% 35% |
| 1   | D     | 40     | 38% 18% • 8% 35%  |
| 1   | E     | 40     | 32% 20% 5% 8% 35% |
| 1   | F     | 40     | 32% 20% 5% 8% 35% |
| 1   | G     | 40     | 32% 22% • 8% 35%  |
| 1   | H     | 40     | 38% 12% 15% 35%   |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 12 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:15-A:23, A:29-A:40,<br>B:15-B:37, C:15-C:37,<br>D:15-D:37, E:15-E:37,<br>F:15-F:37, G:15-G:37,<br>H:15-H:24, H:29-H:38 (179) | 1.39              | 3            |

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 2 clusters. No single-model clusters were found.

| Cluster number | Models              |
|----------------|---------------------|
| 1              | 2, 3, 4, 6, 7, 8, 9 |
| 2              | 1, 5, 10            |

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3072 atoms, of which 1584 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called P3(40).

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |
| 1   | B     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |
| 1   | C     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |
| 1   | D     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |
| 1   | E     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |
| 1   | F     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |
| 1   | G     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |
| 1   | H     | 26       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 384   | 121 | 198 | 31 | 33 | 1 |       |

There are 8 discrepancies between the modelled and reference sequences:

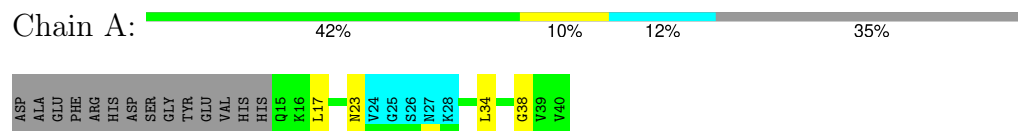
| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| A     | 23      | ASN      | ASP    | variant | UNP P05067 |
| B     | 23      | ASN      | ASP    | variant | UNP P05067 |
| C     | 23      | ASN      | ASP    | variant | UNP P05067 |
| D     | 23      | ASN      | ASP    | variant | UNP P05067 |
| E     | 23      | ASN      | ASP    | variant | UNP P05067 |
| F     | 23      | ASN      | ASP    | variant | UNP P05067 |
| G     | 23      | ASN      | ASP    | variant | UNP P05067 |
| H     | 23      | ASN      | ASP    | variant | UNP P05067 |

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

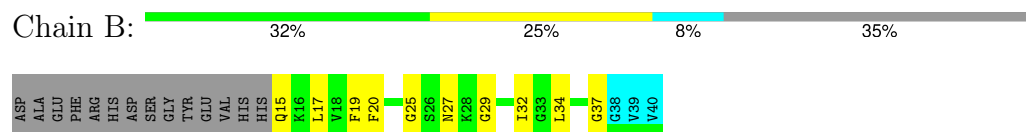
### 4.1 Average score per residue in the NMR ensemble

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.

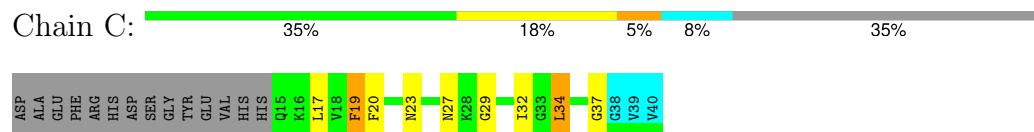
- Molecule 1: P3(40)



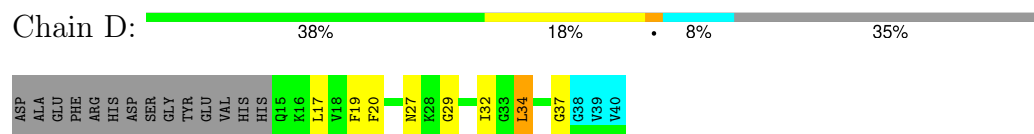
- Molecule 1: P3(40)



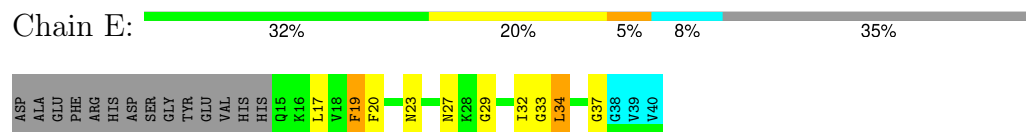
- Molecule 1: P3(40)



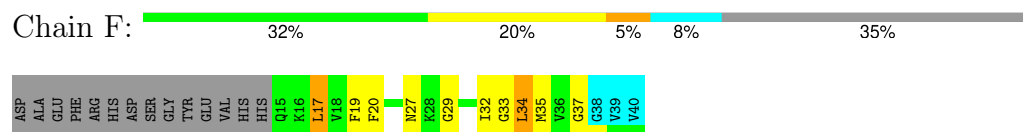
- Molecule 1: P3(40)



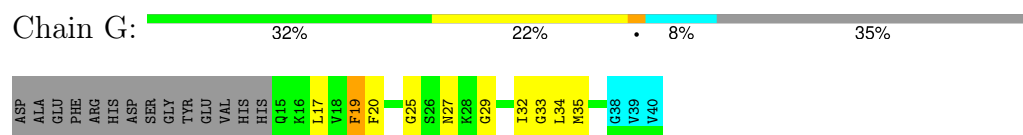
- Molecule 1: P3(40)



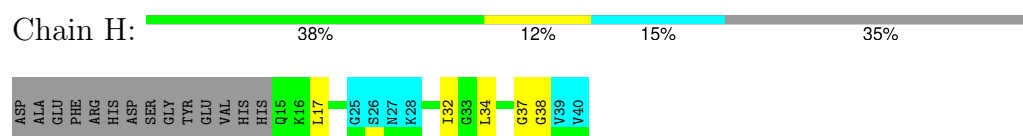
- Molecule 1: P3(40)



- Molecule 1: P3(40)



- Molecule 1: P3(40)

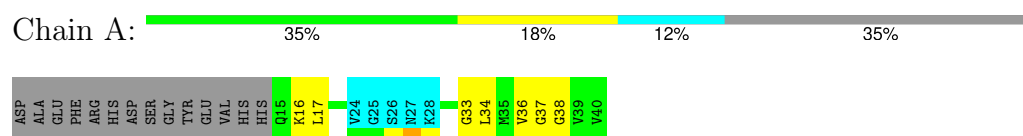


## 4.2 Scores per residue for each member of the ensemble

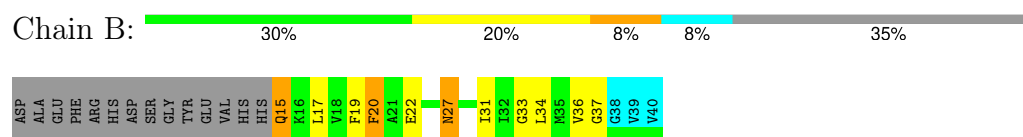
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

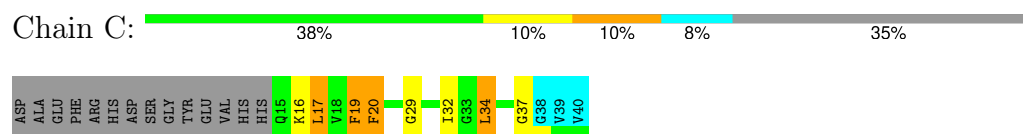
- Molecule 1: P3(40)



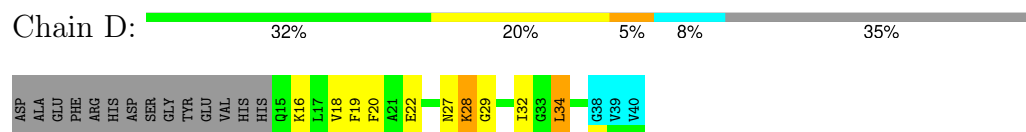
- Molecule 1: P3(40)



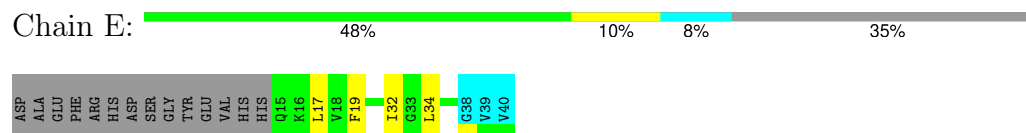
- Molecule 1: P3(40)



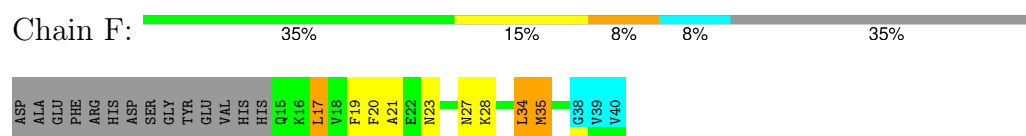
- Molecule 1: P3(40)



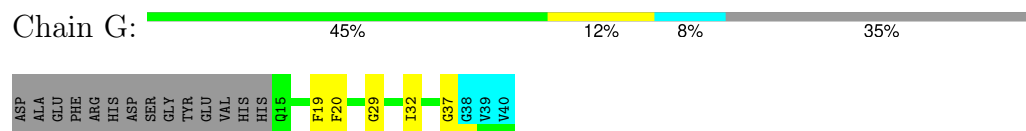
- Molecule 1: P3(40)



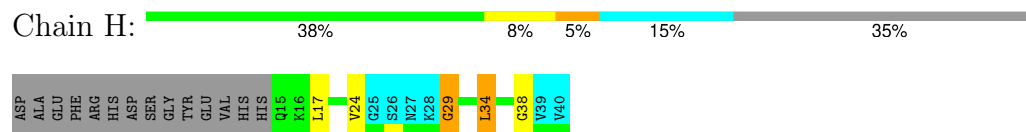
- Molecule 1: P3(40)



- Molecule 1: P3(40)

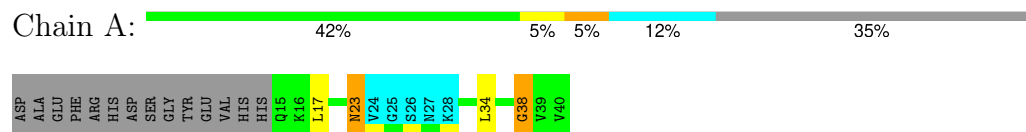


- Molecule 1: P3(40)

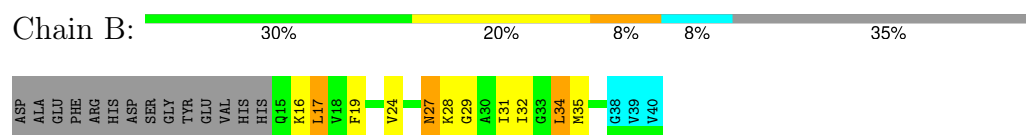


#### 4.2.2 Score per residue for model 2

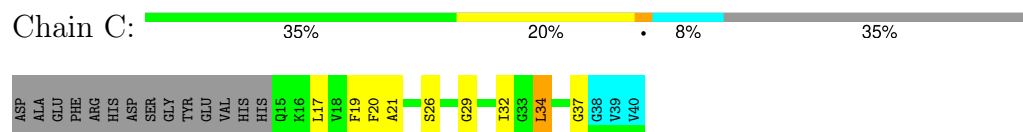
- Molecule 1: P3(40)



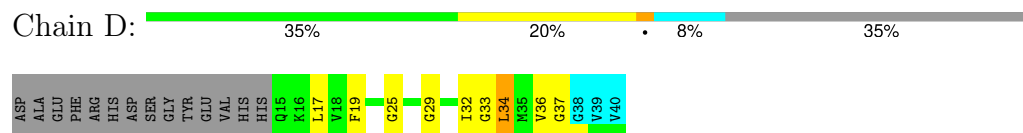
- Molecule 1: P3(40)



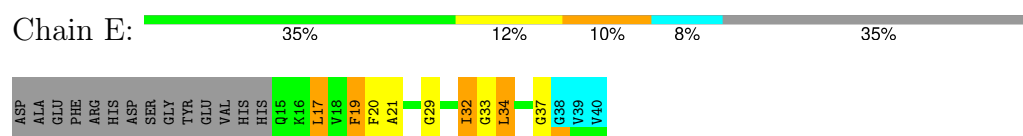
- Molecule 1: P3(40)



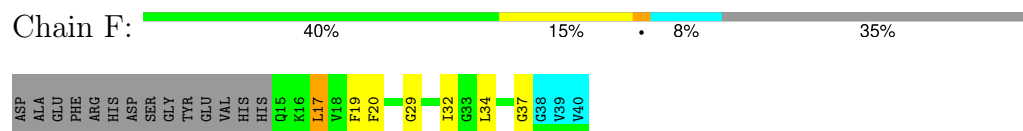
- Molecule 1: P3(40)



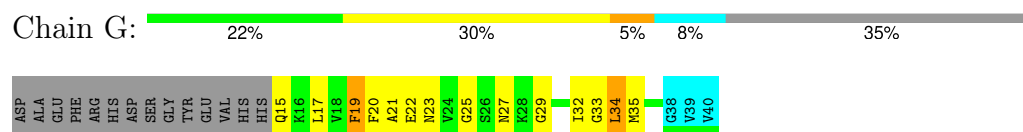
- Molecule 1: P3(40)



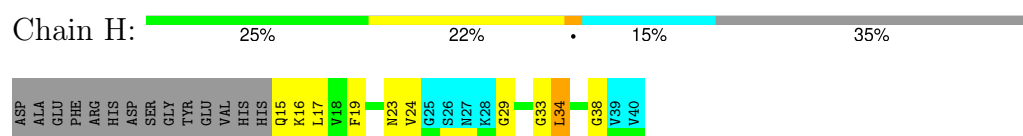
- Molecule 1: P3(40)



- Molecule 1: P3(40)

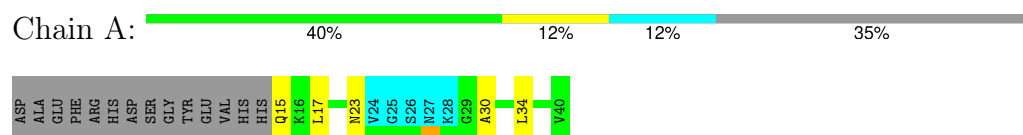


- Molecule 1: P3(40)



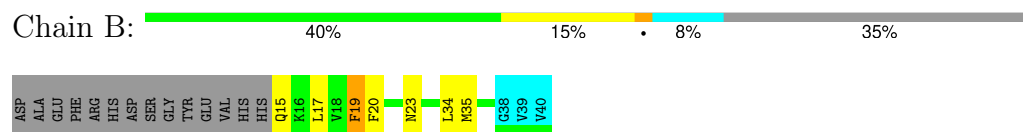
#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: P3(40)

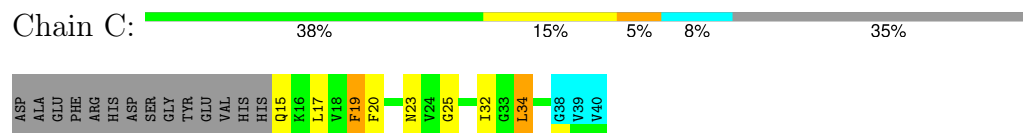


- Molecule 1: P3(40)

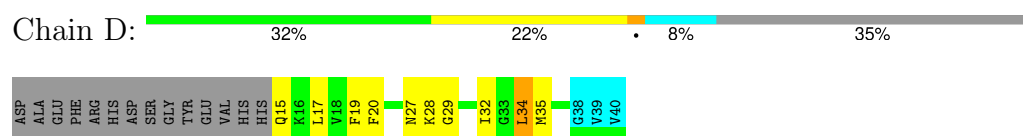




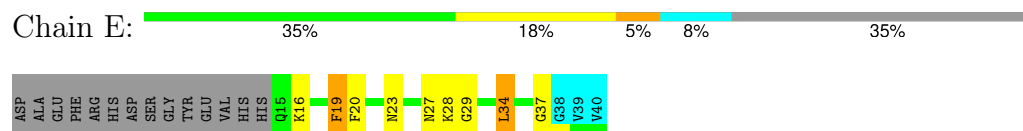
- Molecule 1: P3(40)



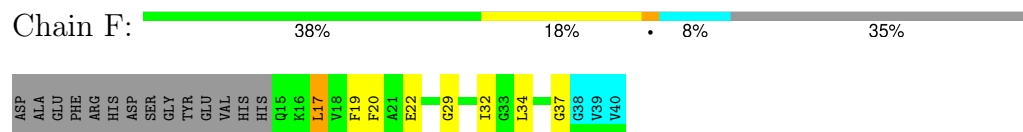
- Molecule 1: P3(40)



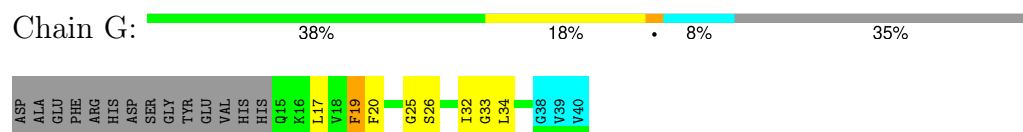
- Molecule 1: P3(40)



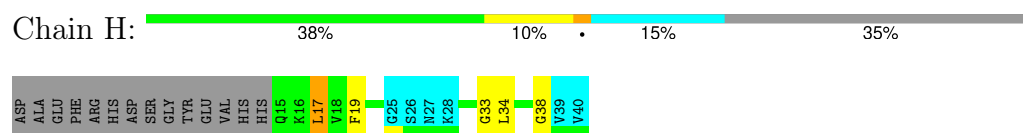
- Molecule 1: P3(40)



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- Molecule 1: P3(40)



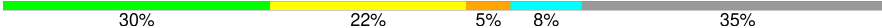
#### 4.2.4 Score per residue for model 4

- Molecule 1: P3(40)

Chain A: 

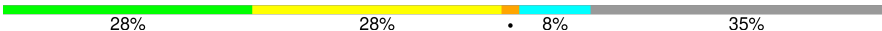


• Molecule 1: P3(40)

Chain B: 




• Molecule 1: P3(40)

Chain C: 




• Molecule 1: P3(40)

Chain D: 




• Molecule 1: P3(40)

Chain E: 




• Molecule 1: P3(40)

Chain F: 



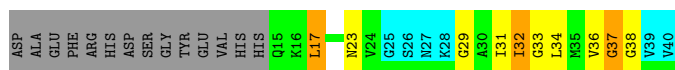
• Molecule 1: P3(40)

Chain G: 



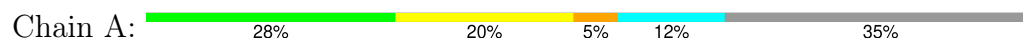
• Molecule 1: P3(40)

Chain H: 

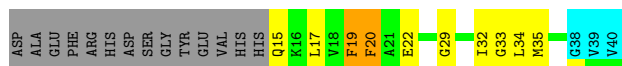
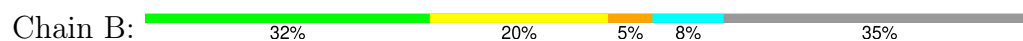


#### 4.2.5 Score per residue for model 5

- Molecule 1: P3(40)



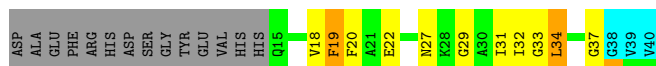
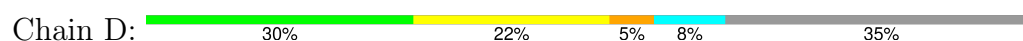
- Molecule 1: P3(40)



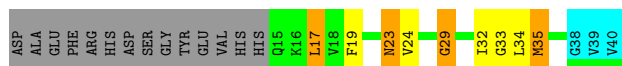
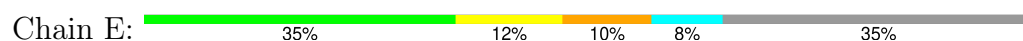
- Molecule 1: P3(40)



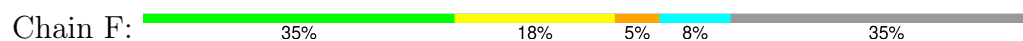
- Molecule 1: P3(40)



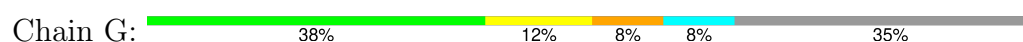
- Molecule 1: P3(40)

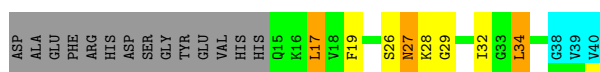


- Molecule 1: P3(40)

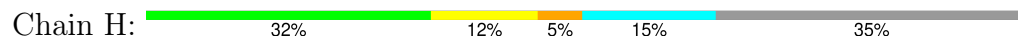


- Molecule 1: P3(40)



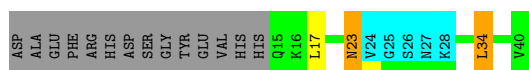


- Molecule 1: P3(40)

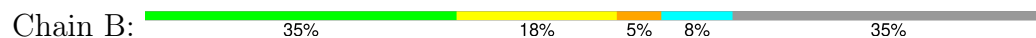


#### 4.2.6 Score per residue for model 6

- Molecule 1: P3(40)



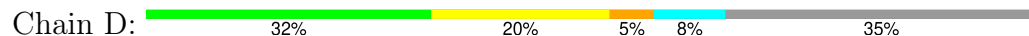
- Molecule 1: P3(40)



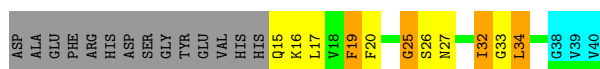
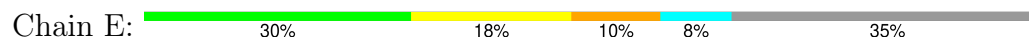
- Molecule 1: P3(40)



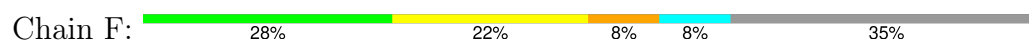
- Molecule 1: P3(40)



- Molecule 1: P3(40)



- Molecule 1: P3(40)

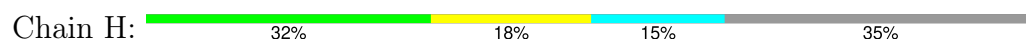




- Molecule 1: P3(40)

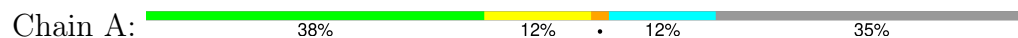


- Molecule 1: P3(40)

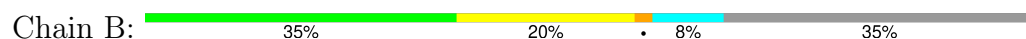


#### 4.2.7 Score per residue for model 7

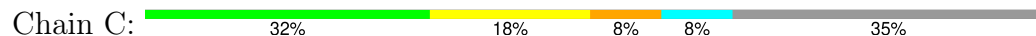
- Molecule 1: P3(40)



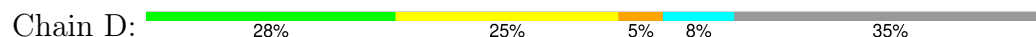
- Molecule 1: P3(40)



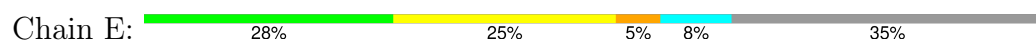
- Molecule 1: P3(40)



- Molecule 1: P3(40)



- Molecule 1: P3(40)





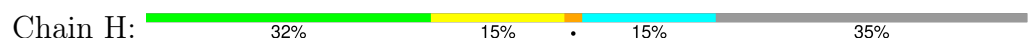
- Molecule 1: P3(40)



- Molecule 1: P3(40)

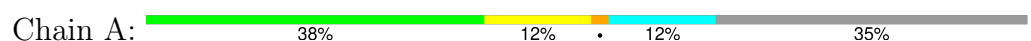


- Molecule 1: P3(40)



#### 4.2.8 Score per residue for model 8

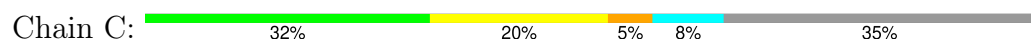
- Molecule 1: P3(40)



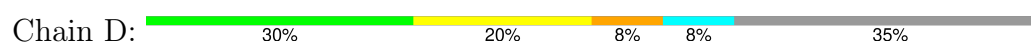
- Molecule 1: P3(40)



- Molecule 1: P3(40)

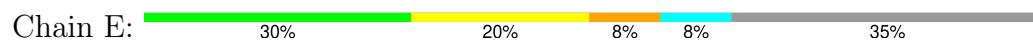


- Molecule 1: P3(40)

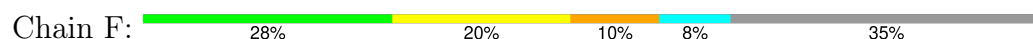




- Molecule 1: P3(40)



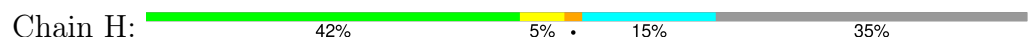
- Molecule 1: P3(40)



- Molecule 1: P3(40)

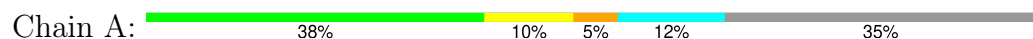


- Molecule 1: P3(40)



#### 4.2.9 Score per residue for model 9

- Molecule 1: P3(40)



- Molecule 1: P3(40)

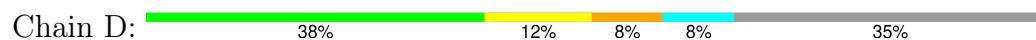


- Molecule 1: P3(40)

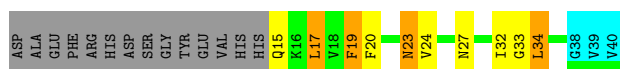
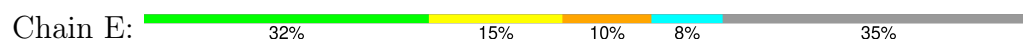




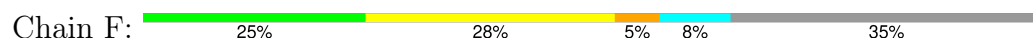
- Molecule 1: P3(40)



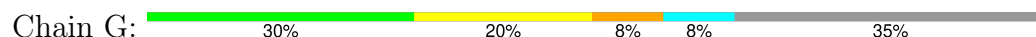
- Molecule 1: P3(40)



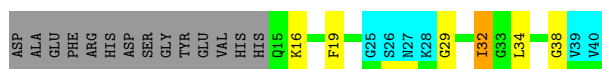
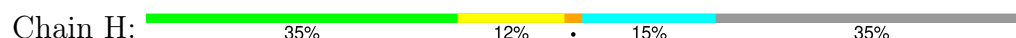
- Molecule 1: P3(40)



- Molecule 1: P3(40)



- Molecule 1: P3(40)

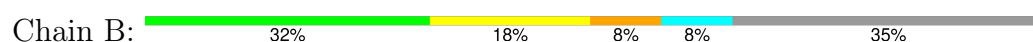


#### 4.2.10 Score per residue for model 10

- Molecule 1: P3(40)



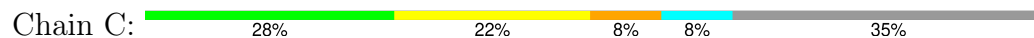
- Molecule 1: P3(40)



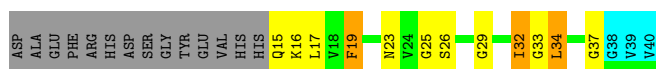
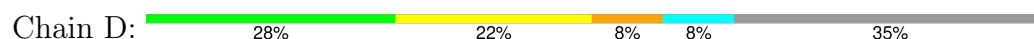




• Molecule 1: P3(40)



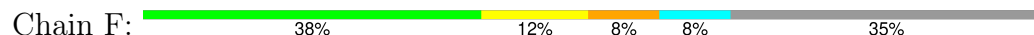
• Molecule 1: P3(40)



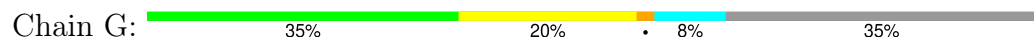
• Molecule 1: P3(40)



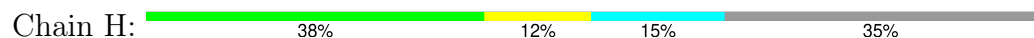
• Molecule 1: P3(40)



• Molecule 1: P3(40)



• Molecule 1: P3(40)



## 5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 10 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| XPLOR-NIH     | refinement     | 2.28.1  |

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                       | 74             |
| Number of shifts mapped to atoms             | 74             |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 3%             |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

## 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     | 152   | 162      | 161      | 4±2     |
| 1   | B     | 167   | 177      | 176      | 11±4    |
| 1   | C     | 167   | 177      | 176      | 12±3    |
| 1   | D     | 167   | 177      | 176      | 13±2    |
| 1   | E     | 167   | 177      | 176      | 14±4    |
| 1   | F     | 167   | 177      | 176      | 12±4    |
| 1   | G     | 167   | 177      | 176      | 14±5    |
| 1   | H     | 144   | 153      | 152      | 8±3     |
| All | All   | 12980 | 13770    | 13690    | 680     |

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 25.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:H:17:LEU:N    | 1:H:17:LEU:HD23 | 0.83     | 1.88        | 4      | 1     |
| 1:D:34:LEU:HD12 | 1:D:34:LEU:O    | 0.83     | 1.74        | 3      | 1     |
| 1:F:33:GLY:C    | 1:F:34:LEU:HD23 | 0.83     | 1.94        | 4      | 2     |
| 1:F:17:LEU:HD23 | 1:F:17:LEU:N    | 0.82     | 1.88        | 1      | 1     |
| 1:E:34:LEU:HD12 | 1:E:34:LEU:N    | 0.82     | 1.90        | 6      | 3     |
| 1:G:17:LEU:N    | 1:G:17:LEU:HD23 | 0.81     | 1.90        | 10     | 1     |
| 1:D:34:LEU:HD12 | 1:D:34:LEU:N    | 0.80     | 1.90        | 10     | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:C:34:LEU:N    | 1:C:34:LEU:HD12 | 0.80     | 1.89        | 6      | 1     |
| 1:E:33:GLY:C    | 1:E:34:LEU:HD23 | 0.80     | 1.96        | 4      | 4     |
| 1:C:34:LEU:HD12 | 1:C:34:LEU:H    | 0.80     | 1.37        | 6      | 1     |
| 1:D:33:GLY:C    | 1:D:34:LEU:HD23 | 0.80     | 1.96        | 5      | 3     |
| 1:E:34:LEU:N    | 1:E:34:LEU:HD23 | 0.80     | 1.90        | 7      | 1     |
| 1:G:17:LEU:HD12 | 1:G:17:LEU:N    | 0.79     | 1.91        | 5      | 1     |
| 1:F:34:LEU:HD12 | 1:F:34:LEU:N    | 0.78     | 1.94        | 8      | 1     |
| 1:C:33:GLY:C    | 1:C:34:LEU:HD23 | 0.76     | 2.00        | 7      | 3     |
| 1:C:19:PHE:CD1  | 1:C:19:PHE:N    | 0.75     | 2.54        | 1      | 1     |
| 1:E:32:ILE:HD13 | 1:E:32:ILE:N    | 0.75     | 1.95        | 2      | 1     |
| 1:B:17:LEU:H    | 1:B:17:LEU:HD23 | 0.75     | 1.41        | 9      | 3     |
| 1:H:17:LEU:HD23 | 1:H:17:LEU:H    | 0.74     | 1.43        | 5      | 2     |
| 1:C:17:LEU:H    | 1:C:17:LEU:HD23 | 0.74     | 1.43        | 6      | 2     |
| 1:A:34:LEU:N    | 1:A:34:LEU:HD23 | 0.74     | 1.97        | 1      | 1     |
| 1:G:34:LEU:C    | 1:G:34:LEU:HD23 | 0.73     | 2.04        | 5      | 1     |
| 1:G:34:LEU:HD12 | 1:G:34:LEU:N    | 0.73     | 1.97        | 9      | 7     |
| 1:G:17:LEU:H    | 1:G:17:LEU:HD23 | 0.73     | 1.44        | 9      | 3     |
| 1:H:32:ILE:HD13 | 1:H:32:ILE:H    | 0.72     | 1.43        | 4      | 3     |
| 1:H:34:LEU:H    | 1:H:34:LEU:HD23 | 0.72     | 1.44        | 6      | 2     |
| 1:B:17:LEU:HD23 | 1:B:17:LEU:N    | 0.72     | 1.98        | 9      | 3     |
| 1:B:17:LEU:C    | 1:B:17:LEU:HD23 | 0.71     | 2.04        | 5      | 1     |
| 1:A:32:ILE:H    | 1:A:32:ILE:HD13 | 0.71     | 1.45        | 10     | 1     |
| 1:D:19:PHE:CD1  | 1:D:20:PHE:N    | 0.70     | 2.59        | 1      | 1     |
| 1:A:34:LEU:HD23 | 1:A:34:LEU:H    | 0.70     | 1.45        | 1      | 1     |
| 1:H:32:ILE:HD13 | 1:H:32:ILE:N    | 0.70     | 2.02        | 9      | 3     |
| 1:B:34:LEU:HD12 | 1:B:34:LEU:N    | 0.69     | 2.01        | 5      | 2     |
| 1:C:17:LEU:HD23 | 1:C:17:LEU:N    | 0.69     | 2.03        | 3      | 2     |
| 1:G:17:LEU:HD23 | 1:G:17:LEU:N    | 0.69     | 2.03        | 8      | 3     |
| 1:H:17:LEU:HD23 | 1:H:17:LEU:N    | 0.69     | 2.03        | 5      | 1     |
| 1:H:34:LEU:HD23 | 1:H:34:LEU:N    | 0.68     | 2.03        | 3      | 2     |
| 1:C:34:LEU:HD23 | 1:C:34:LEU:N    | 0.68     | 2.04        | 8      | 3     |
| 1:E:32:ILE:HD13 | 1:E:32:ILE:H    | 0.68     | 1.47        | 2      | 1     |
| 1:B:19:PHE:CE2  | 1:C:19:PHE:CE1  | 0.67     | 2.81        | 1      | 1     |
| 1:G:19:PHE:CE2  | 1:G:32:ILE:HG21 | 0.67     | 2.24        | 1      | 2     |
| 1:B:19:PHE:CZ   | 1:B:32:ILE:HG21 | 0.66     | 2.26        | 2      | 5     |
| 1:G:17:LEU:HD23 | 1:G:17:LEU:H    | 0.66     | 1.50        | 10     | 1     |
| 1:C:19:PHE:CD1  | 1:C:20:PHE:N    | 0.65     | 2.65        | 4      | 1     |
| 1:E:19:PHE:CD1  | 1:E:19:PHE:C    | 0.64     | 2.71        | 3      | 10    |
| 1:A:32:ILE:HD13 | 1:A:32:ILE:N    | 0.64     | 2.04        | 10     | 1     |
| 1:E:19:PHE:CD2  | 1:F:19:PHE:CE2  | 0.64     | 2.85        | 1      | 1     |
| 1:C:19:PHE:CD2  | 1:D:19:PHE:CB   | 0.64     | 2.81        | 9      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:F:35:MET:SD   | 1:F:35:MET:N    | 0.64     | 2.71        | 4      | 3     |
| 1:G:35:MET:SD   | 1:G:35:MET:N    | 0.63     | 2.72        | 9      | 1     |
| 1:B:15:GLN:N    | 1:B:15:GLN:NE2  | 0.63     | 2.46        | 1      | 1     |
| 1:B:19:PHE:CE2  | 1:C:19:PHE:CD1  | 0.63     | 2.86        | 1      | 2     |
| 1:F:34:LEU:HD23 | 1:F:34:LEU:N    | 0.62     | 2.08        | 7      | 2     |
| 1:G:17:LEU:N    | 1:G:17:LEU:CD2  | 0.62     | 2.62        | 10     | 4     |
| 1:G:33:GLY:C    | 1:G:34:LEU:HD12 | 0.62     | 2.14        | 3      | 6     |
| 1:H:17:LEU:N    | 1:H:17:LEU:CD2  | 0.62     | 2.62        | 4      | 2     |
| 1:G:19:PHE:CZ   | 1:G:32:ILE:HG21 | 0.62     | 2.30        | 10     | 1     |
| 1:E:19:PHE:CB   | 1:F:19:PHE:CD2  | 0.61     | 2.83        | 1      | 1     |
| 1:A:34:LEU:HD12 | 1:A:34:LEU:O    | 0.61     | 1.94        | 6      | 2     |
| 1:H:32:ILE:N    | 1:H:32:ILE:CD1  | 0.61     | 2.63        | 4      | 3     |
| 1:G:19:PHE:C    | 1:G:19:PHE:CD1  | 0.61     | 2.73        | 2      | 4     |
| 1:F:19:PHE:CE2  | 1:G:19:PHE:CD1  | 0.61     | 2.89        | 2      | 5     |
| 1:F:17:LEU:N    | 1:F:17:LEU:CD2  | 0.61     | 2.62        | 1      | 1     |
| 1:F:19:PHE:C    | 1:F:19:PHE:CD1  | 0.61     | 2.74        | 5      | 8     |
| 1:D:19:PHE:O    | 1:D:20:PHE:CD1  | 0.61     | 2.54        | 5      | 2     |
| 1:F:20:PHE:CD1  | 1:F:21:ALA:N    | 0.60     | 2.69        | 5      | 2     |
| 1:E:27:ASN:ND2  | 1:E:28:LYS:N    | 0.60     | 2.48        | 3      | 1     |
| 1:G:32:ILE:HG23 | 1:H:34:LEU:CB   | 0.60     | 2.26        | 6      | 5     |
| 1:D:19:PHE:CE2  | 1:E:19:PHE:CD1  | 0.60     | 2.90        | 6      | 4     |
| 1:B:17:LEU:N    | 1:B:17:LEU:CD2  | 0.60     | 2.64        | 9      | 3     |
| 1:D:34:LEU:HD23 | 1:D:34:LEU:N    | 0.60     | 2.11        | 5      | 2     |
| 1:E:34:LEU:HD12 | 1:E:34:LEU:H    | 0.60     | 1.57        | 3      | 2     |
| 1:B:31:ILE:HD12 | 1:B:31:ILE:C    | 0.59     | 2.18        | 1      | 1     |
| 1:G:32:ILE:HG23 | 1:H:34:LEU:HB3  | 0.59     | 1.74        | 8      | 8     |
| 1:E:27:ASN:ND2  | 1:E:28:LYS:H    | 0.59     | 1.94        | 3      | 1     |
| 1:E:32:ILE:N    | 1:E:32:ILE:CD1  | 0.59     | 2.64        | 2      | 1     |
| 1:E:35:MET:SD   | 1:E:35:MET:N    | 0.59     | 2.75        | 5      | 1     |
| 1:F:19:PHE:CD1  | 1:G:19:PHE:CZ   | 0.59     | 2.91        | 5      | 1     |
| 1:G:17:LEU:N    | 1:G:17:LEU:CD1  | 0.59     | 2.62        | 5      | 1     |
| 1:A:29:GLY:O    | 1:B:37:GLY:N    | 0.59     | 2.34        | 8      | 2     |
| 1:A:32:ILE:N    | 1:A:32:ILE:CD1  | 0.59     | 2.66        | 10     | 1     |
| 1:B:19:PHE:CD1  | 1:C:19:PHE:CE2  | 0.59     | 2.91        | 5      | 1     |
| 1:B:35:MET:SD   | 1:B:35:MET:N    | 0.59     | 2.76        | 9      | 1     |
| 1:A:35:MET:SD   | 1:A:36:VAL:N    | 0.59     | 2.76        | 7      | 1     |
| 1:C:23:ASN:HD22 | 1:C:23:ASN:N    | 0.59     | 1.96        | 4      | 1     |
| 1:A:34:LEU:N    | 1:A:34:LEU:CD2  | 0.59     | 2.65        | 1      | 1     |
| 1:D:19:PHE:C    | 1:D:19:PHE:CD1  | 0.58     | 2.76        | 5      | 6     |
| 1:C:19:PHE:C    | 1:C:19:PHE:CD1  | 0.58     | 2.75        | 6      | 4     |
| 1:B:19:PHE:CZ   | 1:C:19:PHE:CD1  | 0.58     | 2.92        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:H:34:LEU:N    | 1:H:34:LEU:CD2  | 0.58     | 2.65        | 6      | 2     |
| 1:E:23:ASN:HD22 | 1:E:23:ASN:N    | 0.58     | 1.97        | 5      | 1     |
| 1:C:37:GLY:N    | 1:D:29:GLY:O    | 0.58     | 2.36        | 2      | 6     |
| 1:D:23:ASN:ND2  | 1:D:23:ASN:N    | 0.58     | 2.51        | 9      | 1     |
| 1:C:17:LEU:N    | 1:C:17:LEU:CD2  | 0.58     | 2.67        | 6      | 2     |
| 1:C:20:PHE:N    | 1:C:20:PHE:CD1  | 0.58     | 2.72        | 7      | 6     |
| 1:H:17:LEU:O    | 1:H:17:LEU:HD12 | 0.57     | 1.98        | 3      | 2     |
| 1:A:23:ASN:H    | 1:A:23:ASN:HD22 | 0.57     | 1.41        | 6      | 1     |
| 1:B:27:ASN:HD22 | 1:B:28:LYS:N    | 0.57     | 1.96        | 2      | 1     |
| 1:B:19:PHE:C    | 1:B:19:PHE:CD1  | 0.57     | 2.76        | 10     | 4     |
| 1:D:17:LEU:HD12 | 1:D:17:LEU:O    | 0.57     | 1.99        | 4      | 4     |
| 1:F:27:ASN:HD21 | 1:G:15:GLN:N    | 0.57     | 1.96        | 6      | 1     |
| 1:E:17:LEU:CD1  | 1:F:21:ALA:HB2  | 0.57     | 2.29        | 8      | 1     |
| 1:C:17:LEU:HD12 | 1:C:17:LEU:O    | 0.57     | 1.99        | 1      | 3     |
| 1:F:17:LEU:HD12 | 1:F:17:LEU:O    | 0.57     | 1.99        | 2      | 6     |
| 1:B:17:LEU:HD12 | 1:B:17:LEU:O    | 0.57     | 1.99        | 8      | 3     |
| 1:G:19:PHE:CD1  | 1:G:19:PHE:C    | 0.57     | 2.75        | 6      | 4     |
| 1:B:33:GLY:C    | 1:B:34:LEU:HD12 | 0.57     | 2.19        | 5      | 2     |
| 1:E:20:PHE:CE1  | 1:E:21:ALA:O    | 0.57     | 2.57        | 2      | 1     |
| 1:E:34:LEU:HD23 | 1:E:34:LEU:N    | 0.57     | 2.15        | 2      | 3     |
| 1:E:20:PHE:CD1  | 1:E:21:ALA:N    | 0.57     | 2.73        | 2      | 1     |
| 1:E:34:LEU:N    | 1:E:34:LEU:CD1  | 0.57     | 2.60        | 6      | 3     |
| 1:E:16:LYS:O    | 1:F:22:GLU:N    | 0.57     | 2.38        | 7      | 3     |
| 1:C:20:PHE:CD1  | 1:C:21:ALA:N    | 0.56     | 2.74        | 2      | 1     |
| 1:E:23:ASN:HD22 | 1:E:24:VAL:N    | 0.56     | 1.98        | 9      | 1     |
| 1:E:29:GLY:O    | 1:F:37:GLY:N    | 0.56     | 2.38        | 5      | 2     |
| 1:A:16:LYS:O    | 1:B:22:GLU:N    | 0.56     | 2.38        | 4      | 3     |
| 1:C:34:LEU:HB3  | 1:D:32:ILE:HG23 | 0.56     | 1.76        | 2      | 6     |
| 1:C:23:ASN:N    | 1:C:23:ASN:ND2  | 0.56     | 2.53        | 6      | 2     |
| 1:F:23:ASN:ND2  | 1:F:27:ASN:HD22 | 0.56     | 1.97        | 1      | 1     |
| 1:G:29:GLY:O    | 1:H:37:GLY:N    | 0.56     | 2.39        | 10     | 3     |
| 1:B:27:ASN:ND2  | 1:B:27:ASN:N    | 0.56     | 2.54        | 1      | 1     |
| 1:G:20:PHE:N    | 1:G:20:PHE:CD1  | 0.56     | 2.74        | 10     | 5     |
| 1:E:23:ASN:HD22 | 1:E:24:VAL:H    | 0.56     | 1.43        | 9      | 1     |
| 1:E:37:GLY:N    | 1:F:29:GLY:O    | 0.56     | 2.38        | 4      | 4     |
| 1:E:17:LEU:HD12 | 1:E:17:LEU:O    | 0.56     | 2.00        | 5      | 2     |
| 1:F:17:LEU:HD23 | 1:F:17:LEU:H    | 0.56     | 1.61        | 1      | 1     |
| 1:D:18:VAL:CG1  | 1:D:20:PHE:CZ   | 0.56     | 2.89        | 5      | 1     |
| 1:C:29:GLY:O    | 1:D:37:GLY:N    | 0.55     | 2.39        | 4      | 2     |
| 1:E:34:LEU:HB3  | 1:F:32:ILE:HG23 | 0.55     | 1.77        | 7      | 6     |
| 1:G:20:PHE:CD1  | 1:G:20:PHE:C    | 0.55     | 2.80        | 9      | 3     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:G:29:GLY:O    | 1:H:38:GLY:N    | 0.55     | 2.40        | 1      | 5     |
| 1:D:19:PHE:CD1  | 1:E:19:PHE:CE2  | 0.55     | 2.94        | 10     | 2     |
| 1:C:19:PHE:CD1  | 1:C:19:PHE:C    | 0.55     | 2.80        | 8      | 2     |
| 1:G:19:PHE:CE1  | 1:G:32:ILE:HG21 | 0.55     | 2.36        | 5      | 1     |
| 1:G:20:PHE:CE1  | 1:G:21:ALA:O    | 0.55     | 2.60        | 2      | 1     |
| 1:D:23:ASN:N    | 1:D:23:ASN:HD22 | 0.55     | 2.00        | 9      | 2     |
| 1:E:23:ASN:ND2  | 1:E:24:VAL:N    | 0.55     | 2.55        | 9      | 2     |
| 1:B:20:PHE:CD1  | 1:B:20:PHE:N    | 0.54     | 2.76        | 7      | 7     |
| 1:E:37:GLY:O    | 1:F:28:LYS:N    | 0.54     | 2.40        | 7      | 1     |
| 1:B:27:ASN:N    | 1:B:27:ASN:HD22 | 0.54     | 2.00        | 1      | 1     |
| 1:C:16:LYS:O    | 1:D:22:GLU:N    | 0.54     | 2.40        | 1      | 3     |
| 1:F:20:PHE:CE1  | 1:F:21:ALA:O    | 0.54     | 2.60        | 8      | 5     |
| 1:C:25:GLY:H    | 1:D:15:GLN:NE2  | 0.54     | 2.00        | 3      | 1     |
| 1:G:34:LEU:C    | 1:G:34:LEU:CD2  | 0.54     | 2.73        | 5      | 1     |
| 1:C:23:ASN:N    | 1:C:23:ASN:HD22 | 0.54     | 2.01        | 6      | 1     |
| 1:F:27:ASN:N    | 1:F:27:ASN:OD1  | 0.54     | 2.41        | 6      | 1     |
| 1:D:27:ASN:O    | 1:D:27:ASN:ND2  | 0.54     | 2.40        | 9      | 2     |
| 1:E:15:GLN:NE2  | 1:F:27:ASN:OD1  | 0.54     | 2.41        | 4      | 1     |
| 1:H:23:ASN:OD1  | 1:H:24:VAL:N    | 0.53     | 2.41        | 2      | 1     |
| 1:C:22:GLU:N    | 1:D:16:LYS:O    | 0.53     | 2.38        | 4      | 2     |
| 1:A:38:GLY:N    | 1:B:29:GLY:O    | 0.53     | 2.41        | 5      | 4     |
| 1:D:20:PHE:CE1  | 1:D:21:ALA:O    | 0.53     | 2.61        | 8      | 1     |
| 1:E:15:GLN:OE1  | 1:E:15:GLN:N    | 0.53     | 2.41        | 8      | 1     |
| 1:B:27:ASN:O    | 1:B:29:GLY:N    | 0.53     | 2.41        | 9      | 1     |
| 1:E:23:ASN:HD21 | 1:E:26:SER:N    | 0.53     | 2.02        | 10     | 1     |
| 1:C:19:PHE:CE2  | 1:D:19:PHE:CD2  | 0.53     | 2.96        | 2      | 2     |
| 1:G:33:GLY:O    | 1:H:33:GLY:O    | 0.53     | 2.27        | 3      | 5     |
| 1:C:20:PHE:CE1  | 1:C:21:ALA:O    | 0.53     | 2.61        | 10     | 2     |
| 1:B:19:PHE:CD1  | 1:B:19:PHE:C    | 0.53     | 2.80        | 5      | 5     |
| 1:G:27:ASN:HD22 | 1:G:28:LYS:N    | 0.53     | 2.01        | 9      | 1     |
| 1:D:34:LEU:HD12 | 1:E:32:ILE:HD11 | 0.52     | 1.81        | 2      | 1     |
| 1:G:19:PHE:CD1  | 1:G:19:PHE:O    | 0.52     | 2.62        | 6      | 7     |
| 1:D:19:PHE:CZ   | 1:E:19:PHE:CD1  | 0.52     | 2.97        | 3      | 1     |
| 1:G:27:ASN:OD1  | 1:G:28:LYS:N    | 0.52     | 2.42        | 6      | 1     |
| 1:F:27:ASN:OD1  | 1:F:28:LYS:N    | 0.52     | 2.42        | 1      | 1     |
| 1:G:37:GLY:N    | 1:H:29:GLY:O    | 0.52     | 2.42        | 1      | 2     |
| 1:G:34:LEU:HD23 | 1:G:34:LEU:O    | 0.52     | 2.04        | 5      | 1     |
| 1:C:34:LEU:N    | 1:C:34:LEU:CD2  | 0.52     | 2.70        | 8      | 2     |
| 1:C:22:GLU:O    | 1:D:15:GLN:N    | 0.52     | 2.42        | 10     | 1     |
| 1:E:20:PHE:CD1  | 1:E:20:PHE:N    | 0.52     | 2.77        | 3      | 3     |
| 1:A:37:GLY:N    | 1:B:29:GLY:O    | 0.52     | 2.42        | 7      | 2     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:27:ASN:ND2  | 1:B:27:ASN:H    | 0.52     | 2.00        | 1      | 1     |
| 1:G:34:LEU:HD12 | 1:G:34:LEU:H    | 0.52     | 1.65        | 2      | 1     |
| 1:B:23:ASN:ND2  | 1:C:15:GLN:O    | 0.52     | 2.43        | 4      | 2     |
| 1:D:32:ILE:O    | 1:E:34:LEU:HD12 | 0.52     | 2.04        | 3      | 2     |
| 1:A:33:GLY:O    | 1:B:33:GLY:O    | 0.52     | 2.28        | 5      | 2     |
| 1:C:19:PHE:CE1  | 1:C:32:ILE:HD12 | 0.52     | 2.40        | 2      | 1     |
| 1:F:26:SER:OG   | 1:F:27:ASN:N    | 0.52     | 2.43        | 9      | 2     |
| 1:B:23:ASN:ND2  | 1:B:23:ASN:N    | 0.52     | 2.57        | 4      | 1     |
| 1:B:17:LEU:C    | 1:B:17:LEU:CD2  | 0.51     | 2.75        | 5      | 1     |
| 1:C:32:ILE:HG23 | 1:D:34:LEU:HB3  | 0.51     | 1.83        | 5      | 6     |
| 1:D:31:ILE:C    | 1:D:32:ILE:HD12 | 0.51     | 2.26        | 5      | 2     |
| 1:A:23:ASN:O    | 1:A:23:ASN:ND2  | 0.51     | 2.44        | 2      | 1     |
| 1:G:27:ASN:OD1  | 1:H:15:GLN:NE2  | 0.51     | 2.43        | 5      | 1     |
| 1:G:15:GLN:N    | 1:H:22:GLU:O    | 0.51     | 2.43        | 7      | 1     |
| 1:D:27:ASN:HD21 | 1:E:15:GLN:HE22 | 0.51     | 1.48        | 9      | 1     |
| 1:E:27:ASN:OD1  | 1:E:27:ASN:N    | 0.51     | 2.43        | 9      | 2     |
| 1:F:34:LEU:N    | 1:F:34:LEU:CD2  | 0.51     | 2.73        | 7      | 2     |
| 1:D:27:ASN:HD21 | 1:F:27:ASN:ND2  | 0.51     | 2.04        | 4      | 1     |
| 1:F:20:PHE:CD1  | 1:F:20:PHE:N    | 0.51     | 2.78        | 10     | 2     |
| 1:D:20:PHE:C    | 1:D:20:PHE:CD1  | 0.50     | 2.84        | 4      | 4     |
| 1:E:25:GLY:H    | 1:F:15:GLN:NE2  | 0.50     | 2.05        | 6      | 1     |
| 1:G:22:GLU:N    | 1:H:16:LYS:O    | 0.50     | 2.44        | 2      | 2     |
| 1:B:19:PHE:CD1  | 1:B:19:PHE:N    | 0.50     | 2.80        | 1      | 1     |
| 1:E:32:ILE:HG23 | 1:F:34:LEU:HB3  | 0.50     | 1.82        | 1      | 3     |
| 1:E:20:PHE:C    | 1:E:20:PHE:CD1  | 0.50     | 2.85        | 4      | 3     |
| 1:D:19:PHE:CD1  | 1:D:19:PHE:C    | 0.50     | 2.85        | 6      | 3     |
| 1:E:32:ILE:HG22 | 1:F:34:LEU:CB   | 0.50     | 2.36        | 4      | 4     |
| 1:B:32:ILE:O    | 1:C:34:LEU:HD12 | 0.50     | 2.05        | 6      | 1     |
| 1:C:28:LYS:O    | 1:C:30:ALA:N    | 0.50     | 2.45        | 6      | 1     |
| 1:D:15:GLN:O    | 1:E:23:ASN:ND2  | 0.50     | 2.45        | 3      | 1     |
| 1:B:19:PHE:CD1  | 1:B:19:PHE:O    | 0.50     | 2.65        | 5      | 2     |
| 1:B:15:GLN:N    | 1:B:15:GLN:CD   | 0.50     | 2.65        | 1      | 2     |
| 1:D:18:VAL:CG1  | 1:D:20:PHE:CE2  | 0.50     | 2.94        | 5      | 1     |
| 1:D:34:LEU:N    | 1:D:34:LEU:CD2  | 0.50     | 2.75        | 5      | 1     |
| 1:D:34:LEU:N    | 1:D:34:LEU:CD1  | 0.50     | 2.60        | 10     | 1     |
| 1:A:15:GLN:N    | 1:A:15:GLN:CD   | 0.50     | 2.65        | 9      | 3     |
| 1:G:35:MET:O    | 1:H:31:ILE:O    | 0.50     | 2.30        | 7      | 3     |
| 1:C:15:GLN:NE2  | 1:D:23:ASN:HD22 | 0.49     | 2.05        | 10     | 1     |
| 1:G:20:PHE:CD1  | 1:G:21:ALA:N    | 0.49     | 2.80        | 2      | 1     |
| 1:D:27:ASN:O    | 1:D:29:GLY:N    | 0.49     | 2.45        | 3      | 2     |
| 1:E:34:LEU:CB   | 1:F:32:ILE:HG22 | 0.49     | 2.36        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:E:15:GLN:N    | 1:F:22:GLU:O    | 0.49     | 2.46        | 6      | 1     |
| 1:G:34:LEU:N    | 1:G:34:LEU:CD1  | 0.49     | 2.76        | 3      | 6     |
| 1:B:34:LEU:N    | 1:B:34:LEU:CD1  | 0.49     | 2.72        | 5      | 2     |
| 1:D:34:LEU:O    | 1:E:32:ILE:O    | 0.49     | 2.30        | 9      | 1     |
| 1:A:35:MET:SD   | 1:A:36:VAL:O    | 0.49     | 2.71        | 7      | 1     |
| 1:C:27:ASN:O    | 1:D:15:GLN:NE2  | 0.49     | 2.45        | 6      | 1     |
| 1:G:15:GLN:N    | 1:G:15:GLN:CD   | 0.49     | 2.66        | 2      | 1     |
| 1:D:27:ASN:HD21 | 1:F:27:ASN:HD21 | 0.49     | 1.49        | 4      | 1     |
| 1:E:19:PHE:HB3  | 1:F:19:PHE:CD2  | 0.48     | 2.42        | 1      | 1     |
| 1:F:23:ASN:ND2  | 1:G:15:GLN:O    | 0.48     | 2.46        | 7      | 1     |
| 1:D:27:ASN:C    | 1:D:29:GLY:H    | 0.48     | 2.12        | 5      | 1     |
| 1:D:16:LYS:CB   | 1:D:16:LYS:NZ   | 0.48     | 2.76        | 1      | 1     |
| 1:C:34:LEU:N    | 1:C:34:LEU:CD1  | 0.48     | 2.56        | 6      | 1     |
| 1:G:23:ASN:OD1  | 1:G:24:VAL:N    | 0.48     | 2.47        | 6      | 1     |
| 1:F:32:ILE:O    | 1:G:34:LEU:HD12 | 0.48     | 2.08        | 2      | 1     |
| 1:G:27:ASN:ND2  | 1:G:28:LYS:N    | 0.48     | 2.62        | 9      | 1     |
| 1:H:19:PHE:O    | 1:H:19:PHE:CD1  | 0.48     | 2.67        | 6      | 4     |
| 1:G:29:GLY:O    | 1:H:37:GLY:CA   | 0.48     | 2.62        | 6      | 2     |
| 1:E:17:LEU:HD23 | 1:E:17:LEU:N    | 0.48     | 2.24        | 9      | 2     |
| 1:E:37:GLY:CA   | 1:F:29:GLY:O    | 0.48     | 2.62        | 4      | 3     |
| 1:C:33:GLY:O    | 1:D:33:GLY:O    | 0.48     | 2.32        | 10     | 1     |
| 1:A:34:LEU:HB3  | 1:B:32:ILE:HG23 | 0.47     | 1.84        | 10     | 2     |
| 1:G:16:LYS:NZ   | 1:G:16:LYS:CB   | 0.47     | 2.77        | 6      | 1     |
| 1:C:19:PHE:CE2  | 1:C:34:LEU:HD22 | 0.47     | 2.44        | 1      | 1     |
| 1:C:20:PHE:CD1  | 1:C:20:PHE:N    | 0.47     | 2.82        | 1      | 1     |
| 1:D:19:PHE:CE2  | 1:E:19:PHE:CE1  | 0.47     | 3.03        | 3      | 2     |
| 1:B:23:ASN:N    | 1:B:23:ASN:HD22 | 0.47     | 2.07        | 4      | 1     |
| 1:H:35:MET:N    | 1:H:35:MET:SD   | 0.47     | 2.87        | 5      | 1     |
| 1:C:23:ASN:OD1  | 1:D:15:GLN:NE2  | 0.47     | 2.47        | 6      | 1     |
| 1:C:19:PHE:CD2  | 1:D:19:PHE:HB3  | 0.47     | 2.43        | 9      | 2     |
| 1:F:19:PHE:CD1  | 1:F:19:PHE:C    | 0.47     | 2.84        | 10     | 1     |
| 1:B:19:PHE:CZ   | 1:B:32:ILE:CG2  | 0.47     | 2.97        | 2      | 1     |
| 1:D:15:GLN:N    | 1:D:15:GLN:CD   | 0.47     | 2.68        | 4      | 1     |
| 1:E:33:GLY:O    | 1:F:33:GLY:O    | 0.47     | 2.33        | 4      | 6     |
| 1:A:19:PHE:CD1  | 1:A:19:PHE:O    | 0.47     | 2.67        | 5      | 1     |
| 1:E:27:ASN:N    | 1:E:27:ASN:OD1  | 0.47     | 2.48        | 8      | 1     |
| 1:B:15:GLN:OE1  | 1:C:23:ASN:ND2  | 0.47     | 2.47        | 3      | 1     |
| 1:F:31:ILE:C    | 1:F:32:ILE:HD12 | 0.47     | 2.29        | 6      | 1     |
| 1:G:23:ASN:OD1  | 1:H:15:GLN:NE2  | 0.47     | 2.48        | 2      | 1     |
| 1:C:34:LEU:CB   | 1:D:32:ILE:HG22 | 0.47     | 2.40        | 10     | 1     |
| 1:E:19:PHE:CG   | 1:F:19:PHE:CE2  | 0.46     | 3.04        | 1      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:23:ASN:OD1  | 1:B:23:ASN:N    | 0.46     | 2.48        | 3      | 1     |
| 1:E:29:GLY:O    | 1:F:37:GLY:CA   | 0.46     | 2.64        | 8      | 2     |
| 1:F:19:PHE:CD1  | 1:F:19:PHE:O    | 0.46     | 2.68        | 2      | 2     |
| 1:A:34:LEU:C    | 1:A:35:MET:SD   | 0.46     | 2.94        | 5      | 1     |
| 1:B:15:GLN:N    | 1:C:23:ASN:O    | 0.46     | 2.49        | 9      | 1     |
| 1:B:19:PHE:CE2  | 1:B:32:ILE:HG21 | 0.46     | 2.45        | 10     | 2     |
| 1:B:31:ILE:C    | 1:B:32:ILE:HD12 | 0.46     | 2.31        | 2      | 3     |
| 1:E:19:PHE:CE2  | 1:E:32:ILE:HG21 | 0.46     | 2.45        | 5      | 1     |
| 1:G:22:GLU:N    | 1:G:22:GLU:CD   | 0.46     | 2.69        | 8      | 1     |
| 1:G:36:VAL:HG22 | 1:G:37:GLY:N    | 0.46     | 2.25        | 8      | 1     |
| 1:E:15:GLN:N    | 1:E:15:GLN:CD   | 0.46     | 2.68        | 8      | 1     |
| 1:H:19:PHE:C    | 1:H:19:PHE:CD1  | 0.46     | 2.88        | 9      | 1     |
| 1:D:19:PHE:O    | 1:D:19:PHE:CD1  | 0.46     | 2.69        | 5      | 3     |
| 1:B:23:ASN:ND2  | 1:B:23:ASN:H    | 0.46     | 2.09        | 4      | 1     |
| 1:H:34:LEU:C    | 1:H:35:MET:SD   | 0.46     | 2.94        | 5      | 1     |
| 1:F:26:SER:O    | 1:F:27:ASN:O    | 0.46     | 2.34        | 4      | 1     |
| 1:E:34:LEU:N    | 1:E:34:LEU:CD2  | 0.46     | 2.78        | 4      | 3     |
| 1:H:16:LYS:CB   | 1:H:16:LYS:NZ   | 0.46     | 2.79        | 9      | 1     |
| 1:H:19:PHE:CD1  | 1:H:19:PHE:C    | 0.46     | 2.89        | 6      | 4     |
| 1:E:23:ASN:ND2  | 1:E:24:VAL:H    | 0.45     | 2.09        | 10     | 1     |
| 1:C:36:VAL:CG1  | 1:C:37:GLY:N    | 0.45     | 2.79        | 4      | 1     |
| 1:E:23:ASN:N    | 1:E:23:ASN:OD1  | 0.45     | 2.49        | 3      | 2     |
| 1:C:15:GLN:NE2  | 1:D:24:VAL:H    | 0.45     | 2.09        | 7      | 1     |
| 1:G:35:MET:C    | 1:G:35:MET:SD   | 0.45     | 2.95        | 2      | 1     |
| 1:B:16:LYS:NZ   | 1:C:22:GLU:OE1  | 0.45     | 2.49        | 7      | 1     |
| 1:F:34:LEU:N    | 1:F:34:LEU:CD1  | 0.45     | 2.64        | 8      | 1     |
| 1:A:36:VAL:HG22 | 1:A:37:GLY:N    | 0.45     | 2.26        | 1      | 1     |
| 1:B:19:PHE:CE1  | 1:B:32:ILE:HG21 | 0.45     | 2.46        | 2      | 3     |
| 1:D:36:VAL:HG12 | 1:D:37:GLY:N    | 0.45     | 2.26        | 2      | 1     |
| 1:C:36:VAL:HG12 | 1:C:37:GLY:N    | 0.45     | 2.27        | 4      | 1     |
| 1:D:34:LEU:HD12 | 1:D:34:LEU:H    | 0.45     | 1.72        | 1      | 1     |
| 1:C:29:GLY:O    | 1:D:37:GLY:CA   | 0.45     | 2.65        | 6      | 2     |
| 1:C:23:ASN:N    | 1:C:23:ASN:OD1  | 0.45     | 2.46        | 5      | 1     |
| 1:F:36:VAL:O    | 1:F:36:VAL:HG23 | 0.45     | 2.11        | 9      | 1     |
| 1:H:19:PHE:CD1  | 1:H:19:PHE:O    | 0.45     | 2.70        | 9      | 1     |
| 1:C:31:ILE:C    | 1:C:32:ILE:HD12 | 0.45     | 2.32        | 10     | 1     |
| 1:E:23:ASN:HD21 | 1:E:26:SER:H    | 0.45     | 1.52        | 10     | 1     |
| 1:D:19:PHE:CZ   | 1:E:34:LEU:HD11 | 0.44     | 2.47        | 3      | 1     |
| 1:D:35:MET:SD   | 1:D:35:MET:C    | 0.44     | 2.95        | 3      | 1     |
| 1:B:23:ASN:OD1  | 1:B:26:SER:O    | 0.44     | 2.36        | 7      | 1     |
| 1:G:31:ILE:C    | 1:G:32:ILE:HD12 | 0.44     | 2.33        | 10     | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:E:19:PHE:CD1  | 1:E:19:PHE:O    | 0.44     | 2.71        | 3      | 3     |
| 1:B:19:PHE:O    | 1:B:20:PHE:CD1  | 0.44     | 2.70        | 5      | 1     |
| 1:A:23:ASN:N    | 1:A:23:ASN:OD1  | 0.44     | 2.48        | 5      | 1     |
| 1:A:31:ILE:O    | 1:B:35:MET:O    | 0.44     | 2.36        | 5      | 1     |
| 1:B:23:ASN:OD1  | 1:C:15:GLN:O    | 0.44     | 2.35        | 6      | 1     |
| 1:E:35:MET:C    | 1:E:35:MET:SD   | 0.44     | 2.96        | 8      | 1     |
| 1:G:36:VAL:CG2  | 1:G:37:GLY:N    | 0.44     | 2.80        | 8      | 1     |
| 1:B:25:GLY:O    | 1:B:27:ASN:N    | 0.44     | 2.51        | 9      | 1     |
| 1:C:22:GLU:O    | 1:D:16:LYS:O    | 0.44     | 2.36        | 4      | 1     |
| 1:D:19:PHE:CE1  | 1:E:19:PHE:CE2  | 0.44     | 3.05        | 5      | 1     |
| 1:B:36:VAL:O    | 1:B:37:GLY:O    | 0.44     | 2.36        | 6      | 1     |
| 1:G:28:LYS:CB   | 1:G:28:LYS:NZ   | 0.44     | 2.80        | 8      | 1     |
| 1:C:29:GLY:O    | 1:D:37:GLY:O    | 0.44     | 2.36        | 10     | 1     |
| 1:D:19:PHE:CE2  | 1:D:34:LEU:HD21 | 0.44     | 2.47        | 8      | 1     |
| 1:E:37:GLY:O    | 1:F:29:GLY:O    | 0.44     | 2.36        | 10     | 1     |
| 1:B:36:VAL:HG22 | 1:B:37:GLY:N    | 0.44     | 2.27        | 1      | 2     |
| 1:E:36:VAL:HG12 | 1:E:37:GLY:N    | 0.44     | 2.27        | 4      | 1     |
| 1:C:23:ASN:C    | 1:C:23:ASN:HD22 | 0.44     | 2.16        | 9      | 1     |
| 1:F:31:ILE:HG22 | 1:G:35:MET:CB   | 0.44     | 2.43        | 4      | 1     |
| 1:E:24:VAL:HG12 | 1:E:24:VAL:O    | 0.44     | 2.13        | 5      | 1     |
| 1:C:36:VAL:O    | 1:C:36:VAL:HG23 | 0.44     | 2.12        | 8      | 1     |
| 1:E:26:SER:OG   | 1:E:27:ASN:N    | 0.43     | 2.51        | 6      | 1     |
| 1:B:19:PHE:C    | 1:B:20:PHE:CD1  | 0.43     | 2.92        | 5      | 1     |
| 1:C:27:ASN:C    | 1:C:27:ASN:HD22 | 0.43     | 2.15        | 5      | 1     |
| 1:G:25:GLY:O    | 1:G:26:SER:O    | 0.43     | 2.36        | 4      | 1     |
| 1:H:36:VAL:O    | 1:H:37:GLY:O    | 0.43     | 2.36        | 4      | 1     |
| 1:G:24:VAL:HG13 | 1:G:25:GLY:N    | 0.43     | 2.27        | 6      | 2     |
| 1:D:32:ILE:O    | 1:E:34:LEU:O    | 0.43     | 2.37        | 9      | 1     |
| 1:F:23:ASN:HD21 | 1:F:27:ASN:HD22 | 0.43     | 1.55        | 1      | 1     |
| 1:F:19:PHE:CZ   | 1:G:34:LEU:HD13 | 0.43     | 2.48        | 3      | 2     |
| 1:E:19:PHE:HB3  | 1:F:19:PHE:CG   | 0.43     | 2.48        | 1      | 1     |
| 1:B:34:LEU:HD11 | 1:C:32:ILE:HD11 | 0.43     | 1.90        | 2      | 1     |
| 1:B:27:ASN:HD22 | 1:B:27:ASN:C    | 0.43     | 2.16        | 9      | 1     |
| 1:E:23:ASN:ND2  | 1:E:25:GLY:H    | 0.43     | 2.12        | 10     | 1     |
| 1:C:25:GLY:O    | 1:C:26:SER:OG   | 0.43     | 2.37        | 6      | 1     |
| 1:A:37:GLY:CA   | 1:B:29:GLY:O    | 0.43     | 2.67        | 7      | 1     |
| 1:D:20:PHE:CD1  | 1:D:21:ALA:N    | 0.43     | 2.87        | 8      | 1     |
| 1:B:15:GLN:CD   | 1:B:15:GLN:N    | 0.43     | 2.72        | 5      | 1     |
| 1:C:26:SER:O    | 1:C:27:ASN:O    | 0.43     | 2.36        | 7      | 1     |
| 1:C:32:ILE:HG22 | 1:D:34:LEU:CB   | 0.42     | 2.43        | 2      | 1     |
| 1:F:20:PHE:CD1  | 1:F:20:PHE:C    | 0.42     | 2.91        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:23:ASN:OD1  | 1:A:30:ALA:HB3  | 0.42     | 2.14        | 3      | 1     |
| 1:A:19:PHE:CD1  | 1:A:19:PHE:C    | 0.42     | 2.93        | 5      | 1     |
| 1:G:37:GLY:CA   | 1:H:29:GLY:O    | 0.42     | 2.68        | 9      | 1     |
| 1:F:23:ASN:ND2  | 1:F:27:ASN:ND2  | 0.42     | 2.68        | 1      | 1     |
| 1:E:19:PHE:CZ   | 1:E:32:ILE:HG21 | 0.42     | 2.50        | 5      | 1     |
| 1:E:17:LEU:HD12 | 1:F:21:ALA:HB2  | 0.42     | 1.91        | 8      | 1     |
| 1:G:20:PHE:CD1  | 1:G:20:PHE:O    | 0.42     | 2.73        | 4      | 1     |
| 1:A:37:GLY:O    | 1:A:38:GLY:O    | 0.42     | 2.36        | 5      | 1     |
| 1:E:20:PHE:CD1  | 1:E:20:PHE:C    | 0.42     | 2.92        | 6      | 1     |
| 1:C:15:GLN:HE22 | 1:D:25:GLY:N    | 0.42     | 2.13        | 6      | 1     |
| 1:B:17:LEU:HD23 | 1:B:17:LEU:O    | 0.42     | 2.12        | 5      | 1     |
| 1:D:19:PHE:CD1  | 1:D:19:PHE:O    | 0.42     | 2.73        | 10     | 1     |
| 1:B:31:ILE:C    | 1:B:31:ILE:CD1  | 0.42     | 2.85        | 1      | 1     |
| 1:D:28:LYS:NZ   | 1:D:28:LYS:CB   | 0.42     | 2.82        | 9      | 1     |
| 1:C:15:GLN:NE2  | 1:D:24:VAL:N    | 0.42     | 2.68        | 7      | 1     |
| 1:F:36:VAL:O    | 1:F:37:GLY:O    | 0.42     | 2.38        | 7      | 1     |
| 1:C:19:PHE:CD2  | 1:D:19:PHE:CD1  | 0.41     | 3.08        | 1      | 1     |
| 1:G:19:PHE:CZ   | 1:G:32:ILE:CD1  | 0.41     | 3.03        | 4      | 1     |
| 1:F:19:PHE:CD1  | 1:G:19:PHE:CE2  | 0.41     | 3.08        | 5      | 1     |
| 1:C:19:PHE:C    | 1:C:20:PHE:CD1  | 0.41     | 2.93        | 1      | 1     |
| 1:E:23:ASN:N    | 1:E:23:ASN:ND2  | 0.41     | 2.66        | 5      | 1     |
| 1:E:29:GLY:O    | 1:F:37:GLY:O    | 0.41     | 2.37        | 2      | 1     |
| 1:B:25:GLY:O    | 1:B:26:SER:O    | 0.41     | 2.39        | 10     | 1     |
| 1:F:36:VAL:O    | 1:F:36:VAL:HG13 | 0.41     | 2.16        | 5      | 1     |
| 1:G:29:GLY:O    | 1:H:37:GLY:C    | 0.41     | 2.59        | 6      | 1     |
| 1:C:20:PHE:CD2  | 1:D:18:VAL:HG23 | 0.41     | 2.51        | 1      | 1     |
| 1:C:19:PHE:CE2  | 1:D:19:PHE:CG   | 0.41     | 3.09        | 2      | 1     |
| 1:C:15:GLN:NE2  | 1:C:36:VAL:CG1  | 0.41     | 2.83        | 4      | 1     |
| 1:C:37:GLY:CA   | 1:D:29:GLY:O    | 0.41     | 2.68        | 5      | 1     |
| 1:A:36:VAL:HG12 | 1:A:37:GLY:N    | 0.41     | 2.31        | 8      | 1     |
| 1:B:36:VAL:CG2  | 1:B:37:GLY:N    | 0.41     | 2.83        | 1      | 1     |
| 1:F:19:PHE:CE2  | 1:G:19:PHE:CE1  | 0.41     | 3.09        | 2      | 1     |
| 1:E:19:PHE:CD2  | 1:E:32:ILE:HG21 | 0.41     | 2.50        | 10     | 1     |
| 1:F:19:PHE:CD2  | 1:F:34:LEU:HD22 | 0.41     | 2.51        | 1      | 1     |
| 1:C:19:PHE:CD1  | 1:C:19:PHE:O    | 0.41     | 2.74        | 5      | 1     |
| 1:C:36:VAL:HG22 | 1:C:37:GLY:N    | 0.41     | 2.31        | 5      | 1     |
| 1:B:24:VAL:HG23 | 1:B:25:GLY:N    | 0.41     | 2.30        | 9      | 1     |
| 1:H:36:VAL:HG12 | 1:H:37:GLY:N    | 0.41     | 2.31        | 10     | 1     |
| 1:A:36:VAL:O    | 1:A:36:VAL:HG23 | 0.41     | 2.15        | 9      | 1     |
| 1:B:19:PHE:O    | 1:C:19:PHE:O    | 0.40     | 2.39        | 1      | 1     |
| 1:D:34:LEU:HD12 | 1:D:34:LEU:C    | 0.40     | 2.35        | 3      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:E:20:PHE:CD1  | 1:E:20:PHE:O    | 0.40     | 2.74        | 8      | 1     |
| 1:B:25:GLY:O    | 1:B:26:SER:OG   | 0.40     | 2.39        | 4      | 1     |
| 1:D:27:ASN:CG   | 1:D:28:LYS:H    | 0.40     | 2.19        | 1      | 1     |
| 1:D:36:VAL:CG1  | 1:D:37:GLY:N    | 0.40     | 2.84        | 2      | 1     |
| 1:C:19:PHE:CD2  | 1:C:34:LEU:HD22 | 0.40     | 2.51        | 2      | 1     |
| 1:C:19:PHE:CD1  | 1:D:19:PHE:HB3  | 0.40     | 2.52        | 4      | 1     |
| 1:F:36:VAL:HG22 | 1:F:37:GLY:N    | 0.40     | 2.30        | 10     | 1     |

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

| Mol | Chain | Analysed        | Favoured     | Allowed     | Outliers   | Percentiles |    |
|-----|-------|-----------------|--------------|-------------|------------|-------------|----|
| 1   | A     | 19/40 (48%)     | 17±1 (92±3%) | 1±1 (5±4%)  | 1±0 (3±3%) | 5           | 36 |
| 1   | B     | 22/40 (55%)     | 18±2 (81±8%) | 3±1 (14±6%) | 1±1 (5±5%) | 3           | 24 |
| 1   | C     | 22/40 (55%)     | 18±1 (81±5%) | 3±1 (15±5%) | 1±1 (4±3%) | 4           | 33 |
| 1   | D     | 22/40 (55%)     | 18±1 (82±5%) | 3±1 (13±6%) | 1±1 (5±6%) | 3           | 24 |
| 1   | E     | 22/40 (55%)     | 18±2 (83±8%) | 3±1 (13±6%) | 1±1 (4±4%) | 4           | 33 |
| 1   | F     | 22/40 (55%)     | 18±1 (83±6%) | 3±1 (12±5%) | 1±1 (5±5%) | 2           | 22 |
| 1   | G     | 22/40 (55%)     | 17±1 (79±5%) | 3±1 (15±6%) | 1±1 (6±5%) | 2           | 18 |
| 1   | H     | 19/40 (48%)     | 17±1 (89±5%) | 1±1 (7±5%)  | 1±1 (4±4%) | 4           | 29 |
| All | All   | 1700/3200 (53%) | 1419 (83%)   | 203 (12%)   | 78 (5%)    | 3           | 26 |

All 41 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 38  | GLY  | 4              |
| 1   | G     | 25  | GLY  | 4              |
| 1   | F     | 25  | GLY  | 4              |
| 1   | H     | 29  | GLY  | 3              |
| 1   | C     | 29  | GLY  | 3              |
| 1   | D     | 25  | GLY  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | G     | 26  | SER  | 3              |
| 1   | B     | 25  | GLY  | 3              |
| 1   | E     | 25  | GLY  | 3              |
| 1   | E     | 29  | GLY  | 3              |
| 1   | D     | 28  | LYS  | 2              |
| 1   | H     | 24  | VAL  | 2              |
| 1   | G     | 27  | ASN  | 2              |
| 1   | H     | 38  | GLY  | 2              |
| 1   | B     | 37  | GLY  | 2              |
| 1   | G     | 37  | GLY  | 2              |
| 1   | F     | 24  | VAL  | 2              |
| 1   | G     | 24  | VAL  | 2              |
| 1   | C     | 27  | ASN  | 2              |
| 1   | D     | 26  | SER  | 2              |
| 1   | F     | 26  | SER  | 2              |
| 1   | A     | 29  | GLY  | 2              |
| 1   | B     | 26  | SER  | 2              |
| 1   | B     | 28  | LYS  | 2              |
| 1   | B     | 24  | VAL  | 1              |
| 1   | C     | 26  | SER  | 1              |
| 1   | C     | 28  | LYS  | 1              |
| 1   | F     | 27  | ASN  | 1              |
| 1   | F     | 29  | GLY  | 1              |
| 1   | H     | 37  | GLY  | 1              |
| 1   | C     | 25  | GLY  | 1              |
| 1   | G     | 28  | LYS  | 1              |
| 1   | D     | 27  | ASN  | 1              |
| 1   | D     | 37  | GLY  | 1              |
| 1   | E     | 26  | SER  | 1              |
| 1   | E     | 27  | ASN  | 1              |
| 1   | F     | 37  | GLY  | 1              |
| 1   | B     | 29  | GLY  | 1              |
| 1   | F     | 28  | LYS  | 1              |
| 1   | D     | 24  | VAL  | 1              |
| 1   | D     | 29  | GLY  | 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     | 15/31 (48%)     | 12±1 (83±4%) | 2±1 (17±4%) | 4           | 39 |
| 1   | B     | 17/31 (55%)     | 14±1 (82±7%) | 3±1 (18±7%) | 3           | 36 |
| 1   | C     | 17/31 (55%)     | 14±1 (82±5%) | 3±1 (18±5%) | 3           | 36 |
| 1   | D     | 17/31 (55%)     | 14±1 (84±6%) | 3±1 (16±6%) | 4           | 39 |
| 1   | E     | 17/31 (55%)     | 14±1 (82±5%) | 3±1 (18±5%) | 3           | 37 |
| 1   | F     | 17/31 (55%)     | 14±1 (83±3%) | 3±1 (17±3%) | 4           | 38 |
| 1   | G     | 17/31 (55%)     | 15±1 (88±5%) | 2±1 (12±5%) | 6           | 48 |
| 1   | H     | 14/31 (45%)     | 12±1 (87±7%) | 2±1 (13±7%) | 6           | 47 |
| All | All   | 1310/2480 (53%) | 1097 (84%)   | 213 (16%)   | 4           | 39 |

All 57 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     | 17  | LEU  | 10             |
| 1   | C     | 34  | LEU  | 10             |
| 1   | D     | 34  | LEU  | 10             |
| 1   | E     | 34  | LEU  | 10             |
| 1   | F     | 34  | LEU  | 10             |
| 1   | B     | 34  | LEU  | 9              |
| 1   | A     | 34  | LEU  | 9              |
| 1   | F     | 17  | LEU  | 8              |
| 1   | G     | 19  | PHE  | 8              |
| 1   | C     | 17  | LEU  | 7              |
| 1   | E     | 17  | LEU  | 7              |
| 1   | H     | 17  | LEU  | 7              |
| 1   | D     | 17  | LEU  | 7              |
| 1   | E     | 19  | PHE  | 7              |
| 1   | B     | 17  | LEU  | 6              |
| 1   | C     | 19  | PHE  | 5              |
| 1   | H     | 34  | LEU  | 5              |
| 1   | G     | 17  | LEU  | 5              |
| 1   | G     | 34  | LEU  | 5              |
| 1   | F     | 35  | MET  | 4              |
| 1   | B     | 19  | PHE  | 4              |
| 1   | H     | 32  | ILE  | 4              |
| 1   | B     | 27  | ASN  | 3              |
| 1   | B     | 35  | MET  | 3              |
| 1   | E     | 32  | ILE  | 3              |
| 1   | C     | 23  | ASN  | 3              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | D     | 27  | ASN  | 3              |
| 1   | B     | 20  | PHE  | 2              |
| 1   | C     | 20  | PHE  | 2              |
| 1   | A     | 23  | ASN  | 2              |
| 1   | F     | 20  | PHE  | 2              |
| 1   | A     | 32  | ILE  | 2              |
| 1   | C     | 27  | ASN  | 2              |
| 1   | D     | 19  | PHE  | 2              |
| 1   | E     | 23  | ASN  | 2              |
| 1   | F     | 19  | PHE  | 2              |
| 1   | D     | 23  | ASN  | 2              |
| 1   | D     | 35  | MET  | 2              |
| 1   | B     | 15  | GLN  | 1              |
| 1   | B     | 16  | LYS  | 1              |
| 1   | B     | 23  | ASN  | 1              |
| 1   | H     | 23  | ASN  | 1              |
| 1   | B     | 32  | ILE  | 1              |
| 1   | C     | 28  | LYS  | 1              |
| 1   | C     | 35  | MET  | 1              |
| 1   | E     | 35  | MET  | 1              |
| 1   | H     | 35  | MET  | 1              |
| 1   | F     | 27  | ASN  | 1              |
| 1   | G     | 15  | GLN  | 1              |
| 1   | A     | 35  | MET  | 1              |
| 1   | G     | 27  | ASN  | 1              |
| 1   | A     | 15  | GLN  | 1              |
| 1   | D     | 28  | LYS  | 1              |
| 1   | F     | 23  | ASN  | 1              |
| 1   | G     | 35  | MET  | 1              |
| 1   | D     | 32  | ILE  | 1              |
| 1   | F     | 32  | ILE  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 3% for the well-defined parts and 3% 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                  | 74 |
| Number of shifts mapped to atoms        | 74 |
| 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

No chemical shift referencing corrections were calculated (not enough data).

#### 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 3%, i.e. 68 atoms were assigned a chemical shift out of a possible 2379. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total        | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone  | 32/927 (3%)  | 0/390 (0%)     | 32/358 (9%)     | 0/179 (0%)      |
| Sidechain | 36/1292 (3%) | 0/859 (0%)     | 36/397 (9%)     | 0/36 (0%)       |
| Aromatic  | 0/160 (0%)   | 0/80 (0%)      | 0/80 (0%)       | 0/0 (—%)        |
| Overall   | 68/2379 (3%) | 0/1329 (0%)    | 68/835 (8%)     | 0/215 (0%)      |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 3%, i.e. 74 atoms were assigned a chemical shift out of a possible 2728. 0 out of 56 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total        | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone  | 34/1080 (3%) | 0/456 (0%)     | 34/416 (8%)     | 0/208 (0%)      |
| Sidechain | 40/1488 (3%) | 0/992 (0%)     | 40/456 (9%)     | 0/40 (0%)       |
| Aromatic  | 0/160 (0%)   | 0/80 (0%)      | 0/80 (0%)       | 0/0 (—%)        |
| Overall   | 74/2728 (3%) | 0/1528 (0%)    | 74/952 (8%)     | 0/248 (0%)      |

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

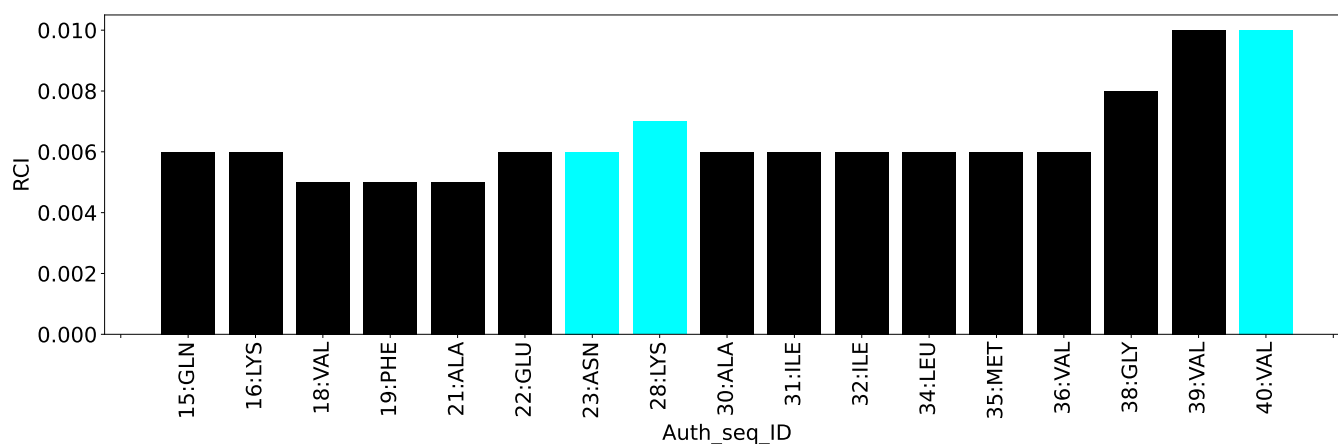
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 217   |
| Intra-residue ( $ i-j =0$ )                              | 0     |
| Sequential ( $ i-j =1$ )                                 | 0     |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 16    |
| Long range ( $ i-j \geq 5$ )                             | 48    |
| Inter-chain  | 65    |
| Hydrogen bond restraints                                 | 88    |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 256   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 1.5   |
| Number of long range restraints per residue <sup>1</sup> | 0.1   |

<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)  | 25.0                                   | 0.2     |
| 0.2-0.5 (Medium) | 80.6                                   | 0.5     |
| >0.5 (Large)     | None                                   | None    |

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

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

| Bins (°)           | Average number of violations per model | Max (°) |
|--------------------|--|---------|
| 1.0-10.0 (Small)   | 64.4                                   | 8.53    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | None                                   | None    |

## 9 Distance violation analysis ⓘ

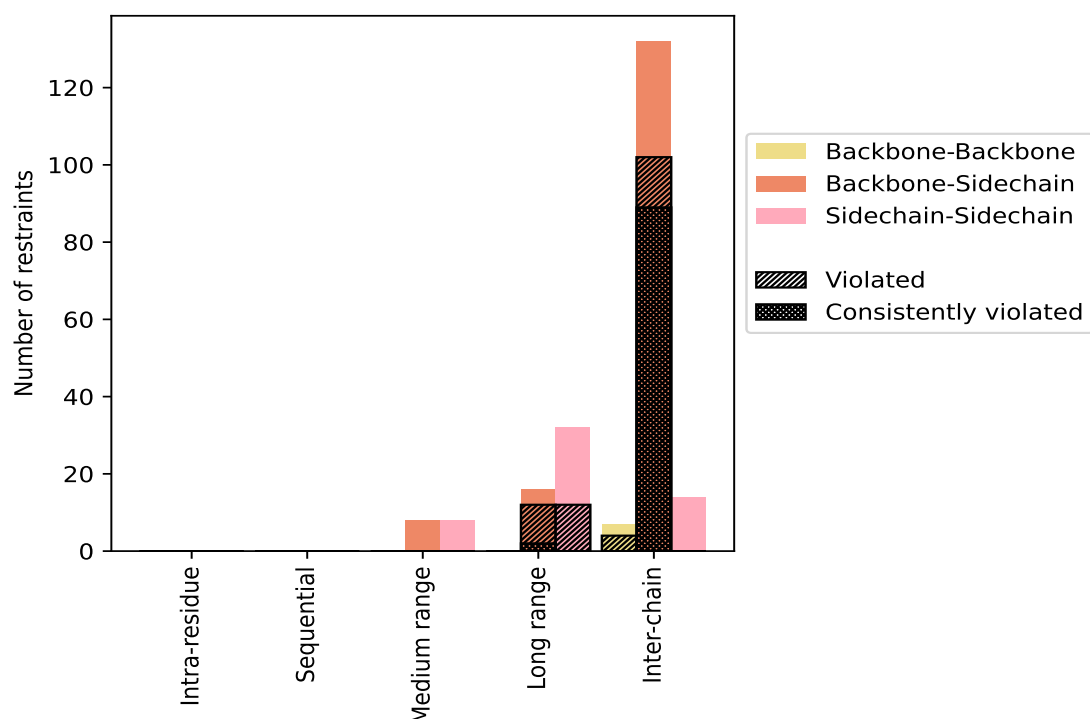
### 9.1 Summary of distance violations ⓘ

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

| Restrains type                         | Count | % <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> |
| Intra-residue ( $ i-j =0$ )            | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sequential ( $ i-j =1$ )               | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Medium range ( $ i-j >1$ & $ i-j <5$ ) | 16    | 7.4            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 8     | 3.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                    | 8     | 3.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Long range ( $ i-j \geq 5$ )           | 48    | 22.1           | 24                    | 50.0           | 11.1           | 2                                  | 4.2            | 0.9            |
| Backbone-Backbone                      | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 16    | 7.4            | 12                    | 75.0           | 5.5            | 2                                  | 12.5           | 0.9            |
| Sidechain-Sidechain                    | 32    | 14.7           | 12                    | 37.5           | 5.5            | 0                                  | 0.0            | 0.0            |
| Inter-chain                            | 65    | 30.0           | 18                    | 27.7           | 8.3            | 2                                  | 3.1            | 0.9            |
| Backbone-Backbone                      | 7     | 3.2            | 4                     | 57.1           | 1.8            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 44    | 20.3           | 14                    | 31.8           | 6.5            | 2                                  | 4.5            | 0.9            |
| Sidechain-Sidechain                    | 14    | 6.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Hydrogen bond                          | 88    | 40.6           | 88                    | 100.0          | 40.6           | 87                                 | 98.9           | 40.1           |
| Disulfide bond                         | 0     | 0.0            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Total                                  | 217   | 100.0          | 130                   | 59.9           | 59.9           | 91                                 | 41.9           | 41.9           |
| Backbone-Backbone                      | 7     | 3.2            | 4                     | 57.1           | 1.8            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                     | 156   | 71.9           | 114                   | 73.1           | 52.5           | 91                                 | 58.3           | 41.9           |
| Sidechain-Sidechain                    | 54    | 24.9           | 12                    | 22.2           | 5.5            | 0                                  | 0.0            | 0.0            |

<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

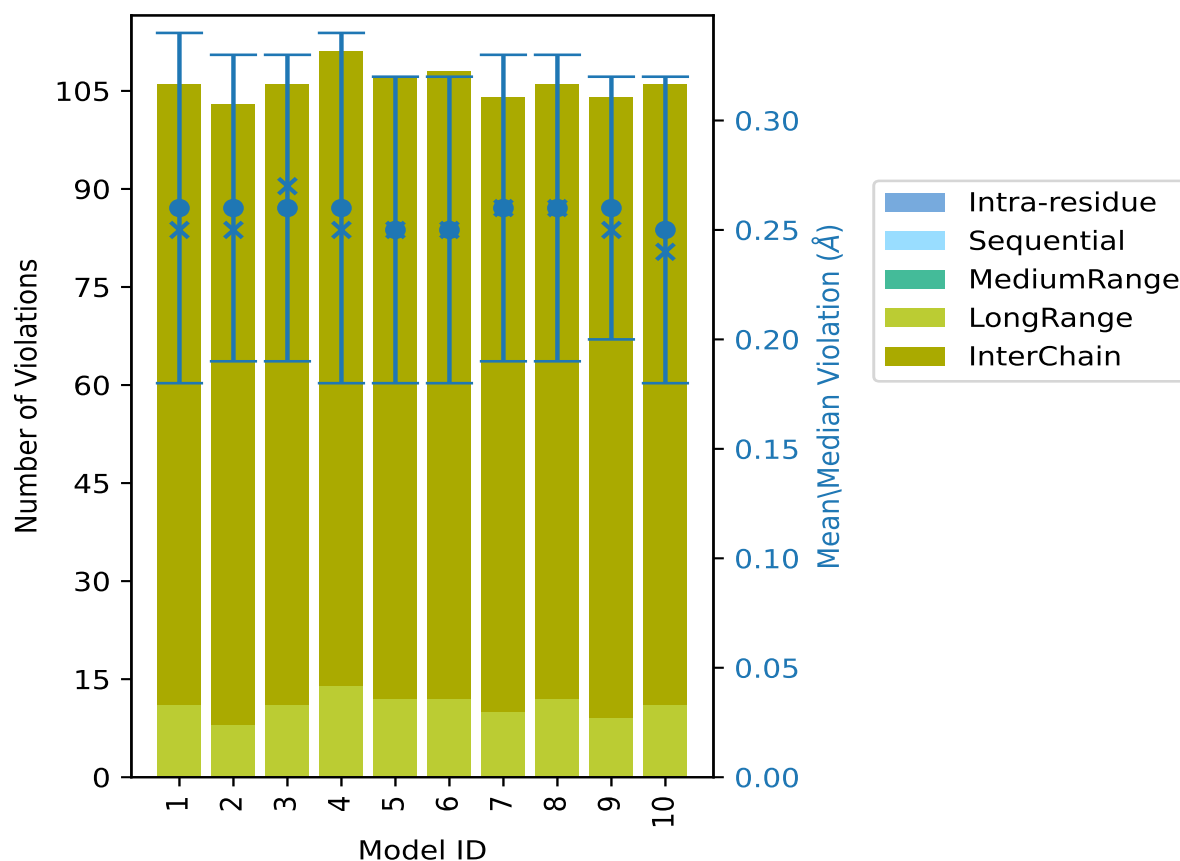
## 9.2 Distance violation statistics for each model [i](#)

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        | 0                    | 0               | 0               | 11              | 95              | 106   | 0.26     | 0.48    | 0.08                | 0.25       |
| 2        | 0                    | 0               | 0               | 8               | 95              | 103   | 0.26     | 0.46    | 0.07                | 0.25       |
| 3        | 0                    | 0               | 0               | 11              | 95              | 106   | 0.26     | 0.4     | 0.07                | 0.27       |
| 4        | 0                    | 0               | 0               | 14              | 97              | 111   | 0.26     | 0.43    | 0.08                | 0.25       |
| 5        | 0                    | 0               | 0               | 12              | 95              | 107   | 0.25     | 0.44    | 0.07                | 0.25       |
| 6        | 0                    | 0               | 0               | 12              | 96              | 108   | 0.25     | 0.41    | 0.07                | 0.25       |
| 7        | 0                    | 0               | 0               | 10              | 94              | 104   | 0.26     | 0.5     | 0.07                | 0.26       |
| 8        | 0                    | 0               | 0               | 12              | 94              | 106   | 0.26     | 0.4     | 0.07                | 0.26       |
| 9        | 0                    | 0               | 0               | 9               | 95              | 104   | 0.26     | 0.42    | 0.06                | 0.25       |
| 10       | 0                    | 0               | 0               | 11              | 95              | 106   | 0.25     | 0.47    | 0.07                | 0.24       |

<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 [i](#)



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 87(IR:0, SQ:0, MR:16, LR:24, IC:47) 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>       | %    |
| 0                             | 0               | 0               | 8               | 9               | 17    | 1                        | 10.0 |
| 0                             | 0               | 0               | 2               | 2               | 4     | 2                        | 20.0 |
| 0                             | 0               | 0               | 1               | 0               | 1     | 3                        | 30.0 |

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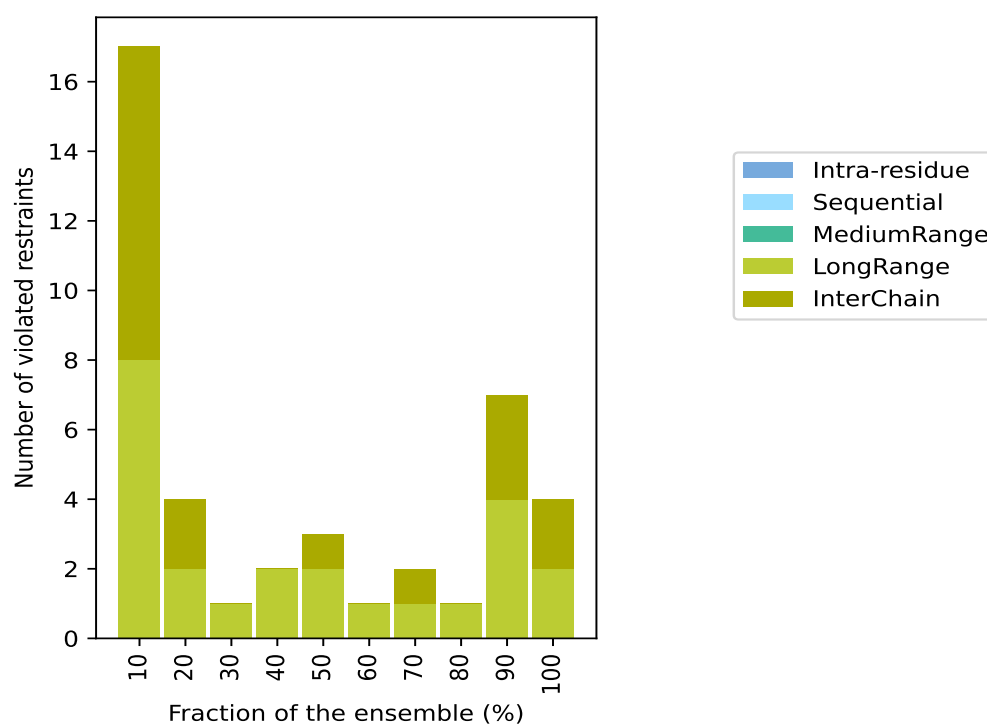
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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>       | %     |
| 0                             | 0               | 0               | 2               | 0               | 2     | 4                        | 40.0  |
| 0                             | 0               | 0               | 2               | 1               | 3     | 5                        | 50.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 6                        | 60.0  |
| 0                             | 0               | 0               | 1               | 1               | 2     | 7                        | 70.0  |
| 0                             | 0               | 0               | 1               | 0               | 1     | 8                        | 80.0  |
| 0                             | 0               | 0               | 4               | 3               | 7     | 9                        | 90.0  |
| 0                             | 0               | 0               | 2               | 2               | 4     | 10                       | 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](#)

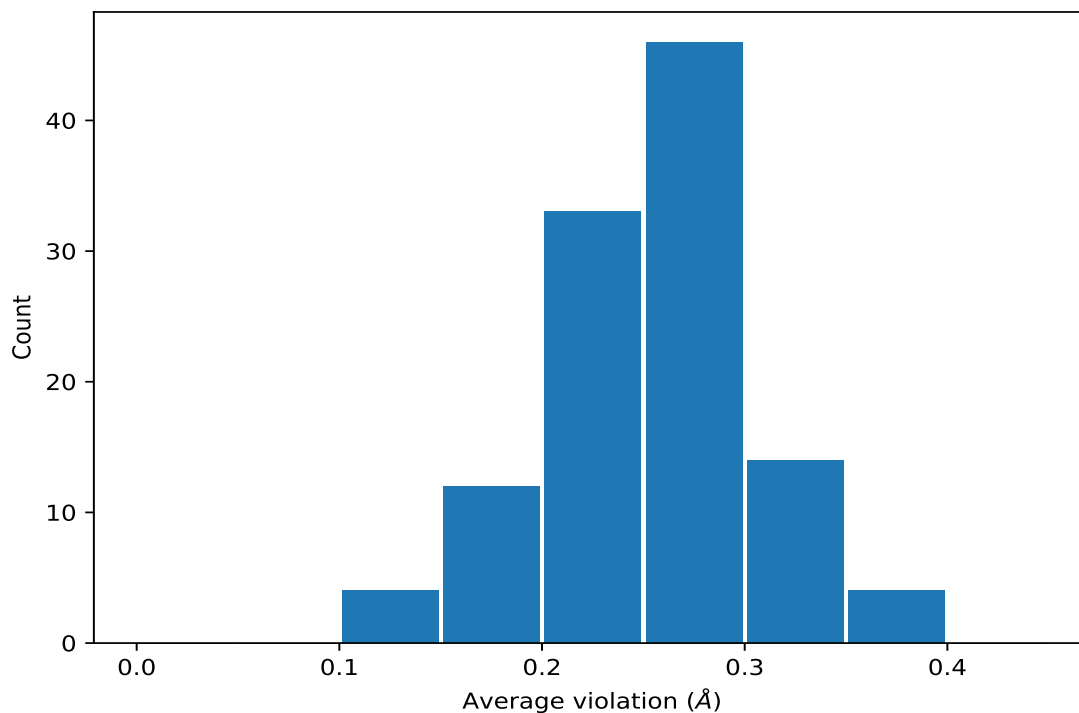


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|---------|---------------|--------------|---------------------|----------|---------------------|------------|
| (2,47)  | 1:31:D:ILE:O  | 1:35:C:MET:H | 10                  | 0.37     | 0.03                | 0.36       |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H | 10                  | 0.37     | 0.06                | 0.37       |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H | 10                  | 0.37     | 0.05                | 0.38       |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H | 10                  | 0.36     | 0.03                | 0.36       |
| (2,49)  | 1:31:E:ILE:O  | 1:35:F:MET:H | 10                  | 0.35     | 0.04                | 0.36       |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H | 10                  | 0.35     | 0.05                | 0.36       |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H | 10                  | 0.34     | 0.03                | 0.34       |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H | 10                  | 0.34     | 0.05                | 0.34       |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H | 10                  | 0.34     | 0.03                | 0.34       |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H | 10                  | 0.33     | 0.06                | 0.31       |
| (2,43)  | 1:35:D:MET:O  | 1:31:C:ILE:H | 10                  | 0.33     | 0.03                | 0.33       |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N | 10                  | 0.33     | 0.03                | 0.34       |
| (2,51)  | 1:35:F:MET:O  | 1:31:E:ILE:H | 10                  | 0.32     | 0.04                | 0.32       |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N | 10                  | 0.32     | 0.1                 | 0.32       |
| (2,13)  | 1:20:C:PHE:O  | 1:18:D:VAL:H | 10                  | 0.31     | 0.05                | 0.31       |

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| Key     | Atom-1        | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|----------------|---------------------|----------|---------------------|------------|
| (2,15)  | 1:18:D:VAL:O  | 1:20:C:PHE:H   | 10                  | 0.31     | 0.05                | 0.29       |
| (2,46)  | 1:35:C:MET:O  | 1:31:D:ILE:N   | 10                  | 0.31     | 0.03                | 0.31       |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 10                  | 0.3      | 0.02                | 0.3        |
| (2,57)  | 1:31:G:ILE:O  | 1:35:H:MET:H   | 10                  | 0.3      | 0.02                | 0.3        |
| (2,37)  | 1:35:A:MET:O  | 1:31:B:ILE:H   | 10                  | 0.3      | 0.04                | 0.29       |
| (2,56)  | 1:31:F:ILE:O  | 1:35:E:MET:N   | 10                  | 0.3      | 0.03                | 0.3        |
| (2,75)  | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 10                  | 0.3      | 0.05                | 0.29       |
| (2,35)  | 1:35:B:MET:O  | 1:31:A:ILE:H   | 10                  | 0.3      | 0.03                | 0.3        |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 10                  | 0.3      | 0.05                | 0.3        |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 10                  | 0.29     | 0.03                | 0.3        |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 10                  | 0.29     | 0.04                | 0.29       |
| (2,39)  | 1:31:B:ILE:O  | 1:35:A:MET:H   | 10                  | 0.29     | 0.03                | 0.29       |
| (2,42)  | 1:31:C:ILE:O  | 1:35:D:MET:N   | 10                  | 0.29     | 0.06                | 0.31       |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 10                  | 0.29     | 0.03                | 0.29       |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H   | 10                  | 0.29     | 0.03                | 0.29       |
| (2,12)  | 1:20:D:PHE:O  | 1:18:C:VAL:N   | 10                  | 0.29     | 0.04                | 0.28       |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 10                  | 0.28     | 0.06                | 0.3        |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 10                  | 0.28     | 0.1                 | 0.28       |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 10                  | 0.28     | 0.04                | 0.26       |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N   | 10                  | 0.28     | 0.03                | 0.28       |
| (2,27)  | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 10                  | 0.28     | 0.04                | 0.27       |
| (2,22)  | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 10                  | 0.28     | 0.03                | 0.29       |
| (2,67)  | 1:34:C:LEU:O  | 1:32:B:ILE:H   | 10                  | 0.27     | 0.03                | 0.27       |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N   | 10                  | 0.27     | 0.04                | 0.26       |
| (2,17)  | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 10                  | 0.27     | 0.05                | 0.26       |
| (2,52)  | 1:35:F:MET:O  | 1:31:E:ILE:N   | 10                  | 0.27     | 0.03                | 0.27       |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 10                  | 0.26     | 0.04                | 0.27       |
| (2,25)  | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 10                  | 0.26     | 0.02                | 0.26       |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 10                  | 0.26     | 0.11                | 0.24       |
| (2,64)  | 1:31:H:ILE:O  | 1:35:G:MET:N   | 10                  | 0.26     | 0.02                | 0.26       |
| (2,29)  | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 10                  | 0.26     | 0.04                | 0.26       |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 10                  | 0.26     | 0.04                | 0.26       |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 10                  | 0.26     | 0.11                | 0.22       |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N   | 10                  | 0.26     | 0.05                | 0.29       |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 10                  | 0.26     | 0.03                | 0.25       |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 10                  | 0.25     | 0.04                | 0.26       |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 10                  | 0.25     | 0.04                | 0.25       |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 10                  | 0.25     | 0.07                | 0.26       |
| (2,60)  | 1:35:H:MET:O  | 1:31:G:ILE:N   | 10                  | 0.25     | 0.04                | 0.24       |
| (2,58)  | 1:31:G:ILE:O  | 1:35:H:MET:N   | 10                  | 0.25     | 0.03                | 0.24       |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 10                  | 0.25     | 0.05                | 0.25       |
| (2,31)  | 1:18:H:VAL:O  | 1:20:G:PHE:H   | 10                  | 0.24     | 0.04                | 0.26       |

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| Key     | Atom-1        | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|----------------|---------------------|----------|---------------------|------------|
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 10                  | 0.24     | 0.03                | 0.23       |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H   | 10                  | 0.24     | 0.03                | 0.24       |
| (2,73)  | 1:32:D:ILE:O  | 1:34:E:LEU:H   | 10                  | 0.24     | 0.02                | 0.24       |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 10                  | 0.24     | 0.04                | 0.23       |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 10                  | 0.24     | 0.04                | 0.22       |
| (2,62)  | 1:35:G:MET:O  | 1:31:H:ILE:N   | 10                  | 0.24     | 0.02                | 0.24       |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 10                  | 0.24     | 0.02                | 0.24       |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 10                  | 0.24     | 0.04                | 0.24       |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H   | 10                  | 0.23     | 0.03                | 0.24       |
| (2,34)  | 1:31:A:ILE:O  | 1:35:B:MET:N   | 10                  | 0.23     | 0.05                | 0.24       |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 10                  | 0.23     | 0.04                | 0.22       |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 10                  | 0.23     | 0.02                | 0.22       |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 10                  | 0.23     | 0.04                | 0.22       |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 10                  | 0.22     | 0.02                | 0.23       |
| (2,65)  | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 10                  | 0.22     | 0.02                | 0.22       |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 10                  | 0.22     | 0.04                | 0.22       |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 10                  | 0.22     | 0.03                | 0.22       |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 10                  | 0.21     | 0.03                | 0.21       |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 10                  | 0.21     | 0.04                | 0.2        |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N   | 10                  | 0.21     | 0.03                | 0.22       |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 10                  | 0.2      | 0.04                | 0.2        |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N   | 10                  | 0.2      | 0.02                | 0.21       |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 10                  | 0.2      | 0.04                | 0.21       |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 10                  | 0.2      | 0.03                | 0.19       |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 10                  | 0.2      | 0.03                | 0.2        |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 10                  | 0.2      | 0.04                | 0.19       |
| (2,72)  | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 10                  | 0.19     | 0.04                | 0.19       |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 10                  | 0.19     | 0.05                | 0.19       |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 10                  | 0.19     | 0.02                | 0.19       |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 10                  | 0.18     | 0.02                | 0.18       |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 10                  | 0.18     | 0.03                | 0.17       |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 10                  | 0.16     | 0.03                | 0.16       |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 10                  | 0.16     | 0.05                | 0.16       |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 10                  | 0.16     | 0.05                | 0.16       |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 9                   | 0.28     | 0.1                 | 0.26       |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 9                   | 0.27     | 0.09                | 0.25       |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N   | 9                   | 0.26     | 0.08                | 0.27       |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 9                   | 0.26     | 0.09                | 0.2        |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 9                   | 0.23     | 0.09                | 0.19       |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 9                   | 0.23     | 0.07                | 0.22       |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 9                   | 0.18     | 0.05                | 0.19       |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 9                   | 0.17     | 0.03                | 0.17       |

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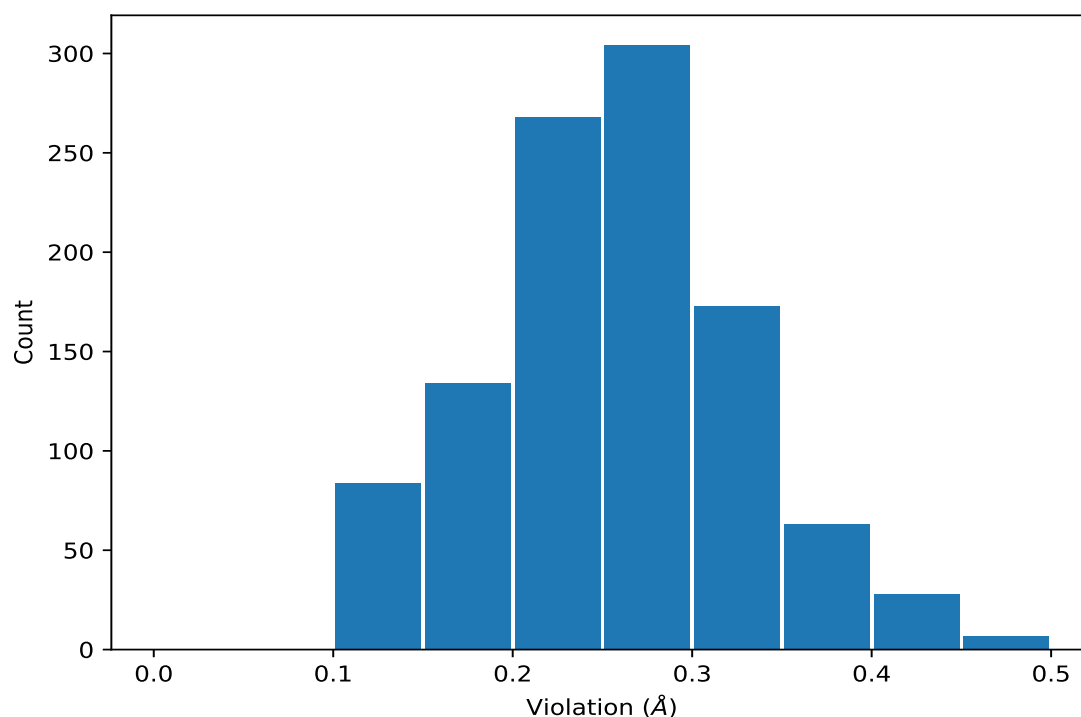
| Key     | Atom-1        | Atom-2         | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|---------|---------------|----------------|---------------------|----------|---------------------|------------|
| (1,55)  | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 8                   | 0.29     | 0.09                | 0.3        |
| (1,39)  | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 7                   | 0.24     | 0.09                | 0.21       |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 7                   | 0.18     | 0.03                | 0.17       |
| (1,23)  | 1:19:C:PHE:CZ | 1:34:C:LEU:CG  | 6                   | 0.34     | 0.09                | 0.35       |
| (1,47)  | 1:19:F:PHE:CZ | 1:34:F:LEU:CG  | 5                   | 0.24     | 0.12                | 0.18       |
| (1,8)   | 1:21:A:ALA:CA | 1:32:A:ILE:CG1 | 5                   | 0.15     | 0.03                | 0.17       |
| (1,101) | 1:33:G:GLY:C  | 1:33:H:GLY:C   | 5                   | 0.15     | 0.02                | 0.17       |
| (1,31)  | 1:19:D:PHE:CZ | 1:34:D:LEU:CG  | 4                   | 0.26     | 0.07                | 0.26       |
| (1,64)  | 1:21:H:ALA:CA | 1:32:H:ILE:CG1 | 4                   | 0.2      | 0.06                | 0.18       |
| (1,15)  | 1:19:B:PHE:CZ | 1:34:B:LEU:CG  | 3                   | 0.22     | 0.12                | 0.14       |
| (1,97)  | 1:19:F:PHE:C  | 1:19:G:PHE:C   | 2                   | 0.26     | 0.01                | 0.26       |
| (1,123) | 1:21:B:ALA:CB | 1:17:A:LEU:N   | 2                   | 0.16     | 0.04                | 0.16       |
| (1,60)  | 1:19:H:PHE:CZ | 1:32:H:ILE:CG2 | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1)   | 1:19:A:PHE:CZ | 1:32:A:ILE:CD1 | 2                   | 0.12     | 0.0                 | 0.12       |

<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

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) |
|---------|---------------|----------------|----------|---------------|
| (1,23)  | 1:19:C:PHE:CZ | 1:34:C:LEU:CG  | 7        | 0.5           |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 7        | 0.48          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 1        | 0.48          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 10       | 0.47          |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 2        | 0.46          |
| (2,47)  | 1:31:D:ILE:O  | 1:35:C:MET:H   | 2        | 0.45          |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 10       | 0.45          |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 5        | 0.44          |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 7        | 0.44          |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 4        | 0.43          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 7        | 0.43          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 2        | 0.43          |
| (2,13)  | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 1        | 0.42          |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 9        | 0.42          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 2        | 0.42          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 9        | 0.42          |
| (1,55)  | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 2        | 0.42          |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 7        | 0.41          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 6        | 0.41          |
| (2,47)  | 1:31:D:ILE:O  | 1:35:C:MET:H   | 6        | 0.41          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 9        | 0.41          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 1        | 0.41          |
| (1,47)  | 1:19:F:PHE:CZ | 1:34:F:LEU:CG  | 5        | 0.41          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 9        | 0.41          |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 3        | 0.4           |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 4        | 0.4           |
| (2,49)  | 1:31:E:ILE:O  | 1:35:F:MET:H   | 5        | 0.4           |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 2        | 0.4           |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 10       | 0.4           |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 1        | 0.4           |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 1        | 0.4           |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 8        | 0.4           |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N   | 5        | 0.4           |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 1        | 0.4           |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 3        | 0.4           |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 6        | 0.39          |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 8        | 0.39          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 4        | 0.39          |
| (2,49)  | 1:31:E:ILE:O  | 1:35:F:MET:H   | 6        | 0.39          |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 1        | 0.39          |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 2        | 0.39          |
| (2,17)  | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 1        | 0.39          |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 3        | 0.39          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 2        | 0.39          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 8        | 0.39          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 6        | 0.39          |
| (1,23)  | 1:19:C:PHE:CZ | 1:34:C:LEU:CG  | 6        | 0.39          |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 9        | 0.38          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 3        | 0.38          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 8        | 0.38          |
| (2,51)  | 1:35:F:MET:O  | 1:31:E:ILE:H   | 5        | 0.38          |
| (2,49)  | 1:31:E:ILE:O  | 1:35:F:MET:H   | 8        | 0.38          |
| (2,47)  | 1:31:D:ILE:O  | 1:35:C:MET:H   | 1        | 0.38          |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 6        | 0.38          |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 4        | 0.38          |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 6        | 0.38          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 4        | 0.38          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 8        | 0.38          |
| (1,55)  | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 6        | 0.38          |
| (1,15)  | 1:19:B:PHE:CZ | 1:34:B:LEU:CG  | 10       | 0.38          |
| (2,75)  | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 4        | 0.37          |
| (2,75)  | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 9        | 0.37          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 9        | 0.37          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N   | 6        | 0.37          |
| (2,47)  | 1:31:D:ILE:O  | 1:35:C:MET:H   | 8        | 0.37          |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 1        | 0.37          |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 10       | 0.37          |
| (2,15)  | 1:18:D:VAL:O  | 1:20:C:PHE:H   | 4        | 0.37          |
| (2,15)  | 1:18:D:VAL:O  | 1:20:C:PHE:H   | 9        | 0.37          |
| (2,12)  | 1:20:D:PHE:O  | 1:18:C:VAL:N   | 4        | 0.37          |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 7        | 0.37          |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 10       | 0.37          |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N   | 2        | 0.37          |
| (1,39)  | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 8        | 0.37          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 1        | 0.37          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 5        | 0.37          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 3        | 0.36          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 8        | 0.36          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 9        | 0.36          |

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| Key    | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|--------|---------------|----------------|----------|---------------|
| (2,51) | 1:35:F:MET:O  | 1:31:E:ILE:H   | 4        | 0.36          |
| (2,49) | 1:31:E:ILE:O  | 1:35:F:MET:H   | 3        | 0.36          |
| (2,49) | 1:31:E:ILE:O  | 1:35:F:MET:H   | 10       | 0.36          |
| (2,48) | 1:31:D:ILE:O  | 1:35:C:MET:N   | 1        | 0.36          |
| (2,47) | 1:31:D:ILE:O  | 1:35:C:MET:H   | 3        | 0.36          |
| (2,47) | 1:31:D:ILE:O  | 1:35:C:MET:H   | 4        | 0.36          |
| (2,47) | 1:31:D:ILE:O  | 1:35:C:MET:H   | 5        | 0.36          |
| (2,43) | 1:35:D:MET:O  | 1:31:C:ILE:H   | 1        | 0.36          |
| (2,43) | 1:35:D:MET:O  | 1:31:C:ILE:H   | 10       | 0.36          |
| (2,42) | 1:31:C:ILE:O  | 1:35:D:MET:N   | 1        | 0.36          |
| (2,41) | 1:31:C:ILE:O  | 1:35:D:MET:H   | 6        | 0.36          |
| (2,37) | 1:35:A:MET:O  | 1:31:B:ILE:H   | 6        | 0.36          |
| (2,33) | 1:31:A:ILE:O  | 1:35:B:MET:H   | 10       | 0.36          |
| (2,21) | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 3        | 0.36          |
| (2,21) | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 9        | 0.36          |
| (2,15) | 1:18:D:VAL:O  | 1:20:C:PHE:H   | 1        | 0.36          |
| (2,13) | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 4        | 0.36          |
| (1,39) | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 3        | 0.36          |
| (1,23) | 1:19:C:PHE:CZ | 1:34:C:LEU:CG  | 3        | 0.36          |
| (2,77) | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 8        | 0.35          |
| (2,61) | 1:35:G:MET:O  | 1:31:H:ILE:H   | 3        | 0.35          |
| (2,56) | 1:31:F:ILE:O  | 1:35:E:MET:N   | 3        | 0.35          |
| (2,55) | 1:31:F:ILE:O  | 1:35:E:MET:H   | 7        | 0.35          |
| (2,53) | 1:35:E:MET:O  | 1:31:F:ILE:H   | 6        | 0.35          |
| (2,51) | 1:35:F:MET:O  | 1:31:E:ILE:H   | 6        | 0.35          |
| (2,49) | 1:31:E:ILE:O  | 1:35:F:MET:H   | 2        | 0.35          |
| (2,47) | 1:31:D:ILE:O  | 1:35:C:MET:H   | 7        | 0.35          |
| (2,47) | 1:31:D:ILE:O  | 1:35:C:MET:H   | 9        | 0.35          |
| (2,47) | 1:31:D:ILE:O  | 1:35:C:MET:H   | 10       | 0.35          |
| (2,46) | 1:35:C:MET:O  | 1:31:D:ILE:N   | 1        | 0.35          |
| (2,46) | 1:35:C:MET:O  | 1:31:D:ILE:N   | 6        | 0.35          |
| (2,45) | 1:35:C:MET:O  | 1:31:D:ILE:H   | 8        | 0.35          |
| (2,43) | 1:35:D:MET:O  | 1:31:C:ILE:H   | 5        | 0.35          |
| (2,27) | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 4        | 0.35          |
| (2,14) | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 1        | 0.35          |
| (2,11) | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 6        | 0.35          |
| (1,55) | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 8        | 0.35          |
| (1,55) | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 9        | 0.35          |
| (1,31) | 1:19:D:PHE:CZ | 1:34:D:LEU:CG  | 1        | 0.35          |
| (1,24) | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 1        | 0.35          |
| (2,75) | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 2        | 0.34          |
| (2,63) | 1:31:H:ILE:O  | 1:35:G:MET:H   | 2        | 0.34          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 4        | 0.34          |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H   | 10       | 0.34          |
| (2,57)  | 1:31:G:ILE:O  | 1:35:H:MET:H   | 2        | 0.34          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 2        | 0.34          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 10       | 0.34          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 5        | 0.34          |
| (2,51)  | 1:35:F:MET:O  | 1:31:E:ILE:H   | 10       | 0.34          |
| (2,49)  | 1:31:E:ILE:O  | 1:35:F:MET:H   | 7        | 0.34          |
| (2,49)  | 1:31:E:ILE:O  | 1:35:F:MET:H   | 9        | 0.34          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N   | 2        | 0.34          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N   | 4        | 0.34          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N   | 8        | 0.34          |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 4        | 0.34          |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 1        | 0.34          |
| (2,43)  | 1:35:D:MET:O  | 1:31:C:ILE:H   | 7        | 0.34          |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 3        | 0.34          |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 4        | 0.34          |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 7        | 0.34          |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 8        | 0.34          |
| (2,39)  | 1:31:B:ILE:O  | 1:35:A:MET:H   | 6        | 0.34          |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N   | 6        | 0.34          |
| (2,37)  | 1:35:A:MET:O  | 1:31:B:ILE:H   | 3        | 0.34          |
| (2,37)  | 1:35:A:MET:O  | 1:31:B:ILE:H   | 8        | 0.34          |
| (2,21)  | 1:20:E:PHE:O  | 1:18:F:VAL:H   | 7        | 0.34          |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 4        | 0.34          |
| (2,15)  | 1:18:D:VAL:O  | 1:20:C:PHE:H   | 2        | 0.34          |
| (2,13)  | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 5        | 0.34          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 1        | 0.34          |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 5        | 0.34          |
| (1,47)  | 1:19:F:PHE:CZ | 1:34:F:LEU:CG  | 10       | 0.34          |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 4        | 0.34          |
| (1,23)  | 1:19:C:PHE:CZ | 1:34:C:LEU:CG  | 4        | 0.34          |
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 1        | 0.33          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 2        | 0.33          |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 9        | 0.33          |
| (2,57)  | 1:31:G:ILE:O  | 1:35:H:MET:H   | 10       | 0.33          |
| (2,56)  | 1:31:F:ILE:O  | 1:35:E:MET:N   | 6        | 0.33          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 5        | 0.33          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 3        | 0.33          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 4        | 0.33          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N   | 3        | 0.33          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N   | 7        | 0.33          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 3        | 0.33          |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 5        | 0.33          |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 7        | 0.33          |
| (2,43)  | 1:35:D:MET:O  | 1:31:C:ILE:H   | 4        | 0.33          |
| (2,43)  | 1:35:D:MET:O  | 1:31:C:ILE:H   | 6        | 0.33          |
| (2,43)  | 1:35:D:MET:O  | 1:31:C:ILE:H   | 8        | 0.33          |
| (2,42)  | 1:31:C:ILE:O  | 1:35:D:MET:N   | 10       | 0.33          |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 5        | 0.33          |
| (2,39)  | 1:31:B:ILE:O  | 1:35:A:MET:H   | 3        | 0.33          |
| (2,35)  | 1:35:B:MET:O  | 1:31:A:ILE:H   | 4        | 0.33          |
| (2,35)  | 1:35:B:MET:O  | 1:31:A:ILE:H   | 7        | 0.33          |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 1        | 0.33          |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 5        | 0.33          |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 10       | 0.33          |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 4        | 0.33          |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 4        | 0.33          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 4        | 0.33          |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 8        | 0.33          |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 1        | 0.33          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 3        | 0.33          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 3        | 0.33          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 9        | 0.33          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 7        | 0.33          |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 4        | 0.32          |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 10       | 0.32          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 8        | 0.32          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 6        | 0.32          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 9        | 0.32          |
| (2,67)  | 1:34:C:LEU:O  | 1:32:B:ILE:H   | 1        | 0.32          |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 7        | 0.32          |
| (2,60)  | 1:35:H:MET:O  | 1:31:G:ILE:N   | 10       | 0.32          |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H   | 5        | 0.32          |
| (2,57)  | 1:31:G:ILE:O  | 1:35:H:MET:H   | 8        | 0.32          |
| (2,56)  | 1:31:F:ILE:O  | 1:35:E:MET:N   | 4        | 0.32          |
| (2,56)  | 1:31:F:ILE:O  | 1:35:E:MET:N   | 8        | 0.32          |
| (2,55)  | 1:31:F:ILE:O  | 1:35:E:MET:H   | 1        | 0.32          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 2        | 0.32          |
| (2,51)  | 1:35:F:MET:O  | 1:31:E:ILE:H   | 3        | 0.32          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N   | 3        | 0.32          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N   | 5        | 0.32          |
| (2,46)  | 1:35:C:MET:O  | 1:31:D:ILE:N   | 4        | 0.32          |
| (2,46)  | 1:35:C:MET:O  | 1:31:D:ILE:N   | 8        | 0.32          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 5        | 0.32          |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 7        | 0.32          |
| (2,43)  | 1:35:D:MET:O  | 1:31:C:ILE:H   | 3        | 0.32          |
| (2,42)  | 1:31:C:ILE:O  | 1:35:D:MET:N   | 6        | 0.32          |
| (2,42)  | 1:31:C:ILE:O  | 1:35:D:MET:N   | 8        | 0.32          |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 6        | 0.32          |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N   | 8        | 0.32          |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 6        | 0.32          |
| (2,29)  | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 5        | 0.32          |
| (2,22)  | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 5        | 0.32          |
| (2,13)  | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 3        | 0.32          |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 1        | 0.32          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 7        | 0.32          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 4        | 0.32          |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 9        | 0.32          |
| (1,34)  | 1:21:E:ALA:CA | 1:32:E:ILE:CD1 | 8        | 0.32          |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 5        | 0.32          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 1        | 0.31          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 2        | 0.31          |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 8        | 0.31          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 3        | 0.31          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 4        | 0.31          |
| (2,67)  | 1:34:C:LEU:O  | 1:32:B:ILE:H   | 3        | 0.31          |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 5        | 0.31          |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 8        | 0.31          |
| (2,57)  | 1:31:G:ILE:O  | 1:35:H:MET:H   | 3        | 0.31          |
| (2,57)  | 1:31:G:ILE:O  | 1:35:H:MET:H   | 7        | 0.31          |
| (2,56)  | 1:31:F:ILE:O  | 1:35:E:MET:N   | 9        | 0.31          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 8        | 0.31          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 9        | 0.31          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 7        | 0.31          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H   | 10       | 0.31          |
| (2,52)  | 1:35:F:MET:O  | 1:31:E:ILE:N   | 4        | 0.31          |
| (2,52)  | 1:35:F:MET:O  | 1:31:E:ILE:N   | 5        | 0.31          |
| (2,51)  | 1:35:F:MET:O  | 1:31:E:ILE:H   | 8        | 0.31          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N   | 6        | 0.31          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N   | 10       | 0.31          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N   | 5        | 0.31          |
| (2,46)  | 1:35:C:MET:O  | 1:31:D:ILE:N   | 2        | 0.31          |
| (2,46)  | 1:35:C:MET:O  | 1:31:D:ILE:N   | 7        | 0.31          |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 9        | 0.31          |
| (2,45)  | 1:35:C:MET:O  | 1:31:D:ILE:H   | 10       | 0.31          |

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| Key    | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|--------|---------------|----------------|----------|---------------|
| (2,42) | 1:31:C:ILE:O  | 1:35:D:MET:N   | 3        | 0.31          |
| (2,42) | 1:31:C:ILE:O  | 1:35:D:MET:N   | 4        | 0.31          |
| (2,42) | 1:31:C:ILE:O  | 1:35:D:MET:N   | 7        | 0.31          |
| (2,41) | 1:31:C:ILE:O  | 1:35:D:MET:H   | 9        | 0.31          |
| (2,39) | 1:31:B:ILE:O  | 1:35:A:MET:H   | 2        | 0.31          |
| (2,39) | 1:31:B:ILE:O  | 1:35:A:MET:H   | 8        | 0.31          |
| (2,38) | 1:35:A:MET:O  | 1:31:B:ILE:N   | 3        | 0.31          |
| (2,37) | 1:35:A:MET:O  | 1:31:B:ILE:H   | 9        | 0.31          |
| (2,36) | 1:35:B:MET:O  | 1:31:A:ILE:N   | 4        | 0.31          |
| (2,35) | 1:35:B:MET:O  | 1:31:A:ILE:H   | 3        | 0.31          |
| (2,35) | 1:35:B:MET:O  | 1:31:A:ILE:H   | 6        | 0.31          |
| (2,35) | 1:35:B:MET:O  | 1:31:A:ILE:H   | 8        | 0.31          |
| (2,27) | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 1        | 0.31          |
| (2,27) | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 7        | 0.31          |
| (2,23) | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 6        | 0.31          |
| (2,22) | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 4        | 0.31          |
| (2,19) | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 8        | 0.31          |
| (2,17) | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 2        | 0.31          |
| (2,16) | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 1        | 0.31          |
| (2,13) | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 6        | 0.31          |
| (2,13) | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 7        | 0.31          |
| (2,12) | 1:20:D:PHE:O  | 1:18:C:VAL:N   | 3        | 0.31          |
| (2,12) | 1:20:D:PHE:O  | 1:18:C:VAL:N   | 7        | 0.31          |
| (1,16) | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 2        | 0.31          |
| (2,86) | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 4        | 0.3           |
| (2,85) | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 5        | 0.3           |
| (2,84) | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 1        | 0.3           |
| (2,75) | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 5        | 0.3           |
| (2,67) | 1:34:C:LEU:O  | 1:32:B:ILE:H   | 8        | 0.3           |
| (2,61) | 1:35:G:MET:O  | 1:31:H:ILE:H   | 2        | 0.3           |
| (2,61) | 1:35:G:MET:O  | 1:31:H:ILE:H   | 6        | 0.3           |
| (2,60) | 1:35:H:MET:O  | 1:31:G:ILE:N   | 5        | 0.3           |
| (2,59) | 1:35:H:MET:O  | 1:31:G:ILE:H   | 1        | 0.3           |
| (2,59) | 1:35:H:MET:O  | 1:31:G:ILE:H   | 2        | 0.3           |
| (2,58) | 1:31:G:ILE:O  | 1:35:H:MET:N   | 10       | 0.3           |
| (2,57) | 1:31:G:ILE:O  | 1:35:H:MET:H   | 1        | 0.3           |
| (2,57) | 1:31:G:ILE:O  | 1:35:H:MET:H   | 5        | 0.3           |
| (2,56) | 1:31:F:ILE:O  | 1:35:E:MET:N   | 2        | 0.3           |
| (2,52) | 1:35:F:MET:O  | 1:31:E:ILE:N   | 10       | 0.3           |
| (2,49) | 1:31:E:ILE:O  | 1:35:F:MET:H   | 4        | 0.3           |
| (2,46) | 1:35:C:MET:O  | 1:31:D:ILE:N   | 3        | 0.3           |
| (2,46) | 1:35:C:MET:O  | 1:31:D:ILE:N   | 5        | 0.3           |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 4        | 0.3           |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 6        | 0.3           |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 8        | 0.3           |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 3        | 0.3           |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N   | 7        | 0.3           |
| (2,35)  | 1:35:B:MET:O  | 1:31:A:ILE:H   | 9        | 0.3           |
| (2,34)  | 1:31:A:ILE:O  | 1:35:B:MET:N   | 6        | 0.3           |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 8        | 0.3           |
| (2,29)  | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 8        | 0.3           |
| (2,29)  | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 9        | 0.3           |
| (2,25)  | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 4        | 0.3           |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 3        | 0.3           |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 5        | 0.3           |
| (2,22)  | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 8        | 0.3           |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 2        | 0.3           |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 3        | 0.3           |
| (2,15)  | 1:18:D:VAL:O  | 1:20:C:PHE:H   | 7        | 0.3           |
| (2,13)  | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 8        | 0.3           |
| (2,11)  | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 5        | 0.3           |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 10       | 0.3           |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N   | 8        | 0.3           |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 10       | 0.3           |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 2        | 0.29          |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 6        | 0.29          |
| (2,75)  | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 7        | 0.29          |
| (2,75)  | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 10       | 0.29          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 2        | 0.29          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 7        | 0.29          |
| (2,64)  | 1:31:H:ILE:O  | 1:35:G:MET:N   | 7        | 0.29          |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 4        | 0.29          |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 10       | 0.29          |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H   | 7        | 0.29          |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H   | 8        | 0.29          |
| (2,56)  | 1:31:F:ILE:O  | 1:35:E:MET:N   | 7        | 0.29          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 2        | 0.29          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 5        | 0.29          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N   | 6        | 0.29          |
| (2,52)  | 1:35:F:MET:O  | 1:31:E:ILE:N   | 3        | 0.29          |
| (2,51)  | 1:35:F:MET:O  | 1:31:E:ILE:H   | 9        | 0.29          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N   | 8        | 0.29          |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 3        | 0.29          |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N   | 10       | 0.29          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 2        | 0.29          |
| (2,39)  | 1:31:B:ILE:O  | 1:35:A:MET:H   | 4        | 0.29          |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N   | 9        | 0.29          |
| (2,37)  | 1:35:A:MET:O  | 1:31:B:ILE:H   | 2        | 0.29          |
| (2,37)  | 1:35:A:MET:O  | 1:31:B:ILE:H   | 7        | 0.29          |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N   | 3        | 0.29          |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N   | 6        | 0.29          |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N   | 8        | 0.29          |
| (2,35)  | 1:35:B:MET:O  | 1:31:A:ILE:H   | 10       | 0.29          |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 3        | 0.29          |
| (2,31)  | 1:18:H:VAL:O  | 1:20:G:PHE:H   | 9        | 0.29          |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 7        | 0.29          |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 9        | 0.29          |
| (2,22)  | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 9        | 0.29          |
| (2,22)  | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 10       | 0.29          |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 4        | 0.29          |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 1        | 0.29          |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 5        | 0.29          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 1        | 0.29          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 3        | 0.29          |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 10       | 0.29          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 6        | 0.29          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 2        | 0.29          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 3        | 0.29          |
| (1,64)  | 1:21:H:ALA:CA | 1:32:H:ILE:CG1 | 7        | 0.29          |
| (1,31)  | 1:19:D:PHE:CZ | 1:34:D:LEU:CG  | 5        | 0.29          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 4        | 0.28          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 1        | 0.28          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 8        | 0.28          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 3        | 0.28          |
| (2,75)  | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 8        | 0.28          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 4        | 0.28          |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 4        | 0.28          |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 9        | 0.28          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 5        | 0.28          |
| (2,64)  | 1:31:H:ILE:O  | 1:35:G:MET:N   | 3        | 0.28          |
| (2,64)  | 1:31:H:ILE:O  | 1:35:G:MET:N   | 5        | 0.28          |
| (2,64)  | 1:31:H:ILE:O  | 1:35:G:MET:N   | 9        | 0.28          |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 1        | 0.28          |
| (2,61)  | 1:35:G:MET:O  | 1:31:H:ILE:H   | 5        | 0.28          |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H   | 3        | 0.28          |
| (2,58)  | 1:31:G:ILE:O  | 1:35:H:MET:N   | 1        | 0.28          |

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| Key    | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|--------|---------------|----------------|----------|---------------|
| (2,58) | 1:31:G:ILE:O  | 1:35:H:MET:N   | 2        | 0.28          |
| (2,58) | 1:31:G:ILE:O  | 1:35:H:MET:N   | 5        | 0.28          |
| (2,57) | 1:31:G:ILE:O  | 1:35:H:MET:H   | 9        | 0.28          |
| (2,52) | 1:35:F:MET:O  | 1:31:E:ILE:N   | 6        | 0.28          |
| (2,51) | 1:35:F:MET:O  | 1:31:E:ILE:H   | 1        | 0.28          |
| (2,51) | 1:35:F:MET:O  | 1:31:E:ILE:H   | 7        | 0.28          |
| (2,49) | 1:31:E:ILE:O  | 1:35:F:MET:H   | 1        | 0.28          |
| (2,42) | 1:31:C:ILE:O  | 1:35:D:MET:N   | 5        | 0.28          |
| (2,40) | 1:31:B:ILE:O  | 1:35:A:MET:N   | 8        | 0.28          |
| (2,39) | 1:31:B:ILE:O  | 1:35:A:MET:H   | 7        | 0.28          |
| (2,39) | 1:31:B:ILE:O  | 1:35:A:MET:H   | 9        | 0.28          |
| (2,37) | 1:35:A:MET:O  | 1:31:B:ILE:H   | 1        | 0.28          |
| (2,37) | 1:35:A:MET:O  | 1:31:B:ILE:H   | 4        | 0.28          |
| (2,36) | 1:35:B:MET:O  | 1:31:A:ILE:N   | 9        | 0.28          |
| (2,35) | 1:35:B:MET:O  | 1:31:A:ILE:H   | 1        | 0.28          |
| (2,29) | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 3        | 0.28          |
| (2,27) | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 9        | 0.28          |
| (2,25) | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 6        | 0.28          |
| (2,25) | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 7        | 0.28          |
| (2,25) | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 9        | 0.28          |
| (2,22) | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 3        | 0.28          |
| (2,17) | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 3        | 0.28          |
| (2,17) | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 6        | 0.28          |
| (2,14) | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 3        | 0.28          |
| (2,14) | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 7        | 0.28          |
| (2,13) | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 9        | 0.28          |
| (2,12) | 1:20:D:PHE:O  | 1:18:C:VAL:N   | 1        | 0.28          |
| (2,12) | 1:20:D:PHE:O  | 1:18:C:VAL:N   | 2        | 0.28          |
| (2,11) | 1:20:D:PHE:O  | 1:18:C:VAL:H   | 8        | 0.28          |
| (2,9)  | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 6        | 0.28          |
| (2,7)  | 1:18:B:VAL:O  | 1:20:A:PHE:H   | 10       | 0.28          |
| (2,3)  | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 2        | 0.28          |
| (2,3)  | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 6        | 0.28          |
| (1,40) | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 5        | 0.28          |
| (1,39) | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 2        | 0.28          |
| (2,85) | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 1        | 0.27          |
| (2,79) | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 6        | 0.27          |
| (2,76) | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 4        | 0.27          |
| (2,75) | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 3        | 0.27          |
| (2,73) | 1:32:D:ILE:O  | 1:34:E:LEU:H   | 8        | 0.27          |
| (2,73) | 1:32:D:ILE:O  | 1:34:E:LEU:H   | 9        | 0.27          |
| (2,71) | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 9        | 0.27          |

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| Key    | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|--------|--------------|--------------|----------|---------------|
| (2,70) | 1:34:B:LEU:O | 1:32:C:ILE:N | 2        | 0.27          |
| (2,67) | 1:34:C:LEU:O | 1:32:B:ILE:H | 2        | 0.27          |
| (2,67) | 1:34:C:LEU:O | 1:32:B:ILE:H | 5        | 0.27          |
| (2,67) | 1:34:C:LEU:O | 1:32:B:ILE:H | 7        | 0.27          |
| (2,65) | 1:32:B:ILE:O | 1:34:C:LEU:H | 1        | 0.27          |
| (2,64) | 1:31:H:ILE:O | 1:35:G:MET:N | 8        | 0.27          |
| (2,62) | 1:35:G:MET:O | 1:31:H:ILE:N | 10       | 0.27          |
| (2,60) | 1:35:H:MET:O | 1:31:G:ILE:N | 1        | 0.27          |
| (2,59) | 1:35:H:MET:O | 1:31:G:ILE:H | 9        | 0.27          |
| (2,57) | 1:31:G:ILE:O | 1:35:H:MET:H | 4        | 0.27          |
| (2,57) | 1:31:G:ILE:O | 1:35:H:MET:H | 6        | 0.27          |
| (2,56) | 1:31:F:ILE:O | 1:35:E:MET:N | 10       | 0.27          |
| (2,54) | 1:35:E:MET:O | 1:31:F:ILE:N | 7        | 0.27          |
| (2,48) | 1:31:D:ILE:O | 1:35:C:MET:N | 10       | 0.27          |
| (2,46) | 1:35:C:MET:O | 1:31:D:ILE:N | 9        | 0.27          |
| (2,43) | 1:35:D:MET:O | 1:31:C:ILE:H | 2        | 0.27          |
| (2,43) | 1:35:D:MET:O | 1:31:C:ILE:H | 9        | 0.27          |
| (2,39) | 1:31:B:ILE:O | 1:35:A:MET:H | 5        | 0.27          |
| (2,38) | 1:35:A:MET:O | 1:31:B:ILE:N | 2        | 0.27          |
| (2,34) | 1:31:A:ILE:O | 1:35:B:MET:N | 3        | 0.27          |
| (2,34) | 1:31:A:ILE:O | 1:35:B:MET:N | 8        | 0.27          |
| (2,31) | 1:18:H:VAL:O | 1:20:G:PHE:H | 3        | 0.27          |
| (2,31) | 1:18:H:VAL:O | 1:20:G:PHE:H | 5        | 0.27          |
| (2,31) | 1:18:H:VAL:O | 1:20:G:PHE:H | 6        | 0.27          |
| (2,31) | 1:18:H:VAL:O | 1:20:G:PHE:H | 8        | 0.27          |
| (2,29) | 1:20:G:PHE:O | 1:18:H:VAL:H | 6        | 0.27          |
| (2,27) | 1:20:H:PHE:O | 1:18:G:VAL:H | 3        | 0.27          |
| (2,27) | 1:20:H:PHE:O | 1:18:G:VAL:H | 6        | 0.27          |
| (2,27) | 1:20:H:PHE:O | 1:18:G:VAL:H | 10       | 0.27          |
| (2,25) | 1:18:G:VAL:O | 1:20:H:PHE:H | 3        | 0.27          |
| (2,23) | 1:18:F:VAL:O | 1:20:E:PHE:H | 4        | 0.27          |
| (2,23) | 1:18:F:VAL:O | 1:20:E:PHE:H | 8        | 0.27          |
| (2,22) | 1:20:E:PHE:O | 1:18:F:VAL:N | 7        | 0.27          |
| (2,20) | 1:20:F:PHE:O | 1:18:E:VAL:N | 10       | 0.27          |
| (2,19) | 1:20:F:PHE:O | 1:18:E:VAL:H | 7        | 0.27          |
| (2,17) | 1:18:E:VAL:O | 1:20:F:PHE:H | 7        | 0.27          |
| (2,15) | 1:18:D:VAL:O | 1:20:C:PHE:H | 3        | 0.27          |
| (2,15) | 1:18:D:VAL:O | 1:20:C:PHE:H | 5        | 0.27          |
| (2,15) | 1:18:D:VAL:O | 1:20:C:PHE:H | 8        | 0.27          |
| (2,15) | 1:18:D:VAL:O | 1:20:C:PHE:H | 10       | 0.27          |
| (2,12) | 1:20:D:PHE:O | 1:18:C:VAL:N | 5        | 0.27          |
| (2,12) | 1:20:D:PHE:O | 1:18:C:VAL:N | 6        | 0.27          |

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| Key     | Atom-1        | Atom-2        | Model ID | Violation (Å) |
|---------|---------------|---------------|----------|---------------|
| (2,12)  | 1:20:D:PHE:O  | 1:18:C:VAL:N  | 10       | 0.27          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H  | 8        | 0.27          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H  | 3        | 0.27          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H  | 4        | 0.27          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H  | 5        | 0.27          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H  | 10       | 0.27          |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H  | 10       | 0.27          |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N  | 3        | 0.27          |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N  | 10       | 0.27          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N  | 4        | 0.27          |
| (1,97)  | 1:19:F:PHE:C  | 1:19:G:PHE:C  | 9        | 0.27          |
| (1,23)  | 1:19:C:PHE:CZ | 1:34:C:LEU:CG | 8        | 0.27          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N  | 4        | 0.26          |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H  | 9        | 0.26          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N  | 2        | 0.26          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H  | 7        | 0.26          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H  | 9        | 0.26          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H  | 10       | 0.26          |
| (2,73)  | 1:32:D:ILE:O  | 1:34:E:LEU:H  | 2        | 0.26          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H  | 2        | 0.26          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H  | 7        | 0.26          |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N  | 7        | 0.26          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H  | 6        | 0.26          |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N  | 1        | 0.26          |
| (2,67)  | 1:34:C:LEU:O  | 1:32:B:ILE:H  | 4        | 0.26          |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H  | 1        | 0.26          |
| (2,62)  | 1:35:G:MET:O  | 1:31:H:ILE:N  | 3        | 0.26          |
| (2,60)  | 1:35:H:MET:O  | 1:31:G:ILE:N  | 2        | 0.26          |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H  | 6        | 0.26          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N  | 10       | 0.26          |
| (2,53)  | 1:35:E:MET:O  | 1:31:F:ILE:H  | 1        | 0.26          |
| (2,52)  | 1:35:F:MET:O  | 1:31:E:ILE:N  | 8        | 0.26          |
| (2,51)  | 1:35:F:MET:O  | 1:31:E:ILE:H  | 2        | 0.26          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N  | 2        | 0.26          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N  | 7        | 0.26          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N  | 9        | 0.26          |
| (2,48)  | 1:31:D:ILE:O  | 1:35:C:MET:N  | 9        | 0.26          |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N  | 4        | 0.26          |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N  | 9        | 0.26          |
| (2,39)  | 1:31:B:ILE:O  | 1:35:A:MET:H  | 1        | 0.26          |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N  | 4        | 0.26          |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N  | 7        | 0.26          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,35)  | 1:35:B:MET:O  | 1:31:A:ILE:H   | 5        | 0.26          |
| (2,27)  | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 2        | 0.26          |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 2        | 0.26          |
| (2,22)  | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 6        | 0.26          |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 6        | 0.26          |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 9        | 0.26          |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 7        | 0.26          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 2        | 0.26          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 7        | 0.26          |
| (2,9)   | 1:18:C:VAL:O  | 1:20:D:PHE:H   | 5        | 0.26          |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 7        | 0.26          |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 8        | 0.26          |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 8        | 0.26          |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 10       | 0.26          |
| (1,97)  | 1:19:F:PHE:C  | 1:19:G:PHE:C   | 8        | 0.26          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 8        | 0.26          |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 4        | 0.26          |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 2        | 0.25          |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 8        | 0.25          |
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 4        | 0.25          |
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 9        | 0.25          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 6        | 0.25          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 7        | 0.25          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 9        | 0.25          |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 3        | 0.25          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 5        | 0.25          |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 2        | 0.25          |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 10       | 0.25          |
| (2,73)  | 1:32:D:ILE:O  | 1:34:E:LEU:H   | 3        | 0.25          |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 8        | 0.25          |
| (2,67)  | 1:34:C:LEU:O  | 1:32:B:ILE:H   | 6        | 0.25          |
| (2,67)  | 1:34:C:LEU:O  | 1:32:B:ILE:H   | 10       | 0.25          |
| (2,64)  | 1:31:H:ILE:O  | 1:35:G:MET:N   | 2        | 0.25          |
| (2,64)  | 1:31:H:ILE:O  | 1:35:G:MET:N   | 6        | 0.25          |
| (2,63)  | 1:31:H:ILE:O  | 1:35:G:MET:H   | 10       | 0.25          |
| (2,62)  | 1:35:G:MET:O  | 1:31:H:ILE:N   | 1        | 0.25          |
| (2,62)  | 1:35:G:MET:O  | 1:31:H:ILE:N   | 5        | 0.25          |
| (2,59)  | 1:35:H:MET:O  | 1:31:G:ILE:H   | 4        | 0.25          |
| (2,56)  | 1:31:F:ILE:O  | 1:35:E:MET:N   | 1        | 0.25          |
| (2,52)  | 1:35:F:MET:O  | 1:31:E:ILE:N   | 1        | 0.25          |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 7        | 0.25          |
| (2,39)  | 1:31:B:ILE:O  | 1:35:A:MET:H   | 10       | 0.25          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N   | 1        | 0.25          |
| (2,37)  | 1:35:A:MET:O  | 1:31:B:ILE:H   | 5        | 0.25          |
| (2,37)  | 1:35:A:MET:O  | 1:31:B:ILE:H   | 10       | 0.25          |
| (2,35)  | 1:35:B:MET:O  | 1:31:A:ILE:H   | 2        | 0.25          |
| (2,34)  | 1:31:A:ILE:O  | 1:35:B:MET:N   | 1        | 0.25          |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 2        | 0.25          |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 3        | 0.25          |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 9        | 0.25          |
| (2,29)  | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 2        | 0.25          |
| (2,29)  | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 7        | 0.25          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 4        | 0.25          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 7        | 0.25          |
| (2,25)  | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 1        | 0.25          |
| (2,25)  | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 5        | 0.25          |
| (2,25)  | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 8        | 0.25          |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 1        | 0.25          |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 3        | 0.25          |
| (2,17)  | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 9        | 0.25          |
| (2,15)  | 1:18:D:VAL:O  | 1:20:C:PHE:H   | 6        | 0.25          |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 6        | 0.25          |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 8        | 0.25          |
| (2,13)  | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 10       | 0.25          |
| (2,12)  | 1:20:D:PHE:O  | 1:18:C:VAL:N   | 9        | 0.25          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 3        | 0.25          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 9        | 0.25          |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H   | 3        | 0.25          |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H   | 5        | 0.25          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H   | 1        | 0.25          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 7        | 0.25          |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 9        | 0.25          |
| (1,55)  | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 3        | 0.25          |
| (1,55)  | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 7        | 0.25          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 5        | 0.25          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 3        | 0.25          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 1        | 0.24          |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 1        | 0.24          |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 6        | 0.24          |
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 5        | 0.24          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 4        | 0.24          |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 5        | 0.24          |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 7        | 0.24          |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 8        | 0.24          |

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| Key    | Atom-1       | Atom-2       | Model ID | Violation (Å) |
|--------|--------------|--------------|----------|---------------|
| (2,76) | 1:34:E:LEU:O | 1:32:D:ILE:N | 9        | 0.24          |
| (2,75) | 1:34:E:LEU:O | 1:32:D:ILE:H | 6        | 0.24          |
| (2,73) | 1:32:D:ILE:O | 1:34:E:LEU:H | 5        | 0.24          |
| (2,73) | 1:32:D:ILE:O | 1:34:E:LEU:H | 10       | 0.24          |
| (2,72) | 1:32:C:ILE:O | 1:34:B:LEU:N | 2        | 0.24          |
| (2,72) | 1:32:C:ILE:O | 1:34:B:LEU:N | 4        | 0.24          |
| (2,72) | 1:32:C:ILE:O | 1:34:B:LEU:N | 9        | 0.24          |
| (2,71) | 1:32:C:ILE:O | 1:34:B:LEU:H | 8        | 0.24          |
| (2,69) | 1:34:B:LEU:O | 1:32:C:ILE:H | 10       | 0.24          |
| (2,68) | 1:34:C:LEU:O | 1:32:B:ILE:N | 3        | 0.24          |
| (2,68) | 1:34:C:LEU:O | 1:32:B:ILE:N | 5        | 0.24          |
| (2,65) | 1:32:B:ILE:O | 1:34:C:LEU:H | 8        | 0.24          |
| (2,64) | 1:31:H:ILE:O | 1:35:G:MET:N | 1        | 0.24          |
| (2,64) | 1:31:H:ILE:O | 1:35:G:MET:N | 4        | 0.24          |
| (2,62) | 1:35:G:MET:O | 1:31:H:ILE:N | 9        | 0.24          |
| (2,60) | 1:35:H:MET:O | 1:31:G:ILE:N | 8        | 0.24          |
| (2,58) | 1:31:G:ILE:O | 1:35:H:MET:N | 3        | 0.24          |
| (2,56) | 1:31:F:ILE:O | 1:35:E:MET:N | 5        | 0.24          |
| (2,50) | 1:31:E:ILE:O | 1:35:F:MET:N | 1        | 0.24          |
| (2,46) | 1:35:C:MET:O | 1:31:D:ILE:N | 10       | 0.24          |
| (2,44) | 1:35:D:MET:O | 1:31:C:ILE:N | 2        | 0.24          |
| (2,34) | 1:31:A:ILE:O | 1:35:B:MET:N | 10       | 0.24          |
| (2,33) | 1:31:A:ILE:O | 1:35:B:MET:H | 9        | 0.24          |
| (2,32) | 1:18:H:VAL:O | 1:20:G:PHE:N | 9        | 0.24          |
| (2,31) | 1:18:H:VAL:O | 1:20:G:PHE:H | 7        | 0.24          |
| (2,30) | 1:20:G:PHE:O | 1:18:H:VAL:N | 8        | 0.24          |
| (2,25) | 1:18:G:VAL:O | 1:20:H:PHE:H | 10       | 0.24          |
| (2,24) | 1:18:F:VAL:O | 1:20:E:PHE:N | 3        | 0.24          |
| (2,24) | 1:18:F:VAL:O | 1:20:E:PHE:N | 4        | 0.24          |
| (2,24) | 1:18:F:VAL:O | 1:20:E:PHE:N | 9        | 0.24          |
| (2,22) | 1:20:E:PHE:O | 1:18:F:VAL:N | 1        | 0.24          |
| (2,21) | 1:20:E:PHE:O | 1:18:F:VAL:H | 2        | 0.24          |
| (2,20) | 1:20:F:PHE:O | 1:18:E:VAL:N | 7        | 0.24          |
| (2,20) | 1:20:F:PHE:O | 1:18:E:VAL:N | 8        | 0.24          |
| (2,18) | 1:18:E:VAL:O | 1:20:F:PHE:N | 2        | 0.24          |
| (2,17) | 1:18:E:VAL:O | 1:20:F:PHE:H | 4        | 0.24          |
| (2,16) | 1:18:D:VAL:O | 1:20:C:PHE:N | 5        | 0.24          |
| (2,12) | 1:20:D:PHE:O | 1:18:C:VAL:N | 8        | 0.24          |
| (2,10) | 1:18:C:VAL:O | 1:20:D:PHE:N | 5        | 0.24          |
| (2,7)  | 1:18:B:VAL:O | 1:20:A:PHE:H | 4        | 0.24          |
| (2,7)  | 1:18:B:VAL:O | 1:20:A:PHE:H | 6        | 0.24          |
| (2,6)  | 1:20:A:PHE:O | 1:18:B:VAL:N | 5        | 0.24          |

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| Key    | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|--------|---------------|----------------|----------|---------------|
| (2,4)  | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 8        | 0.24          |
| (2,3)  | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 5        | 0.24          |
| (2,1)  | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 6        | 0.24          |
| (1,56) | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 5        | 0.24          |
| (1,48) | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 8        | 0.24          |
| (1,24) | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 6        | 0.24          |
| (2,86) | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 10       | 0.23          |
| (2,83) | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 2        | 0.23          |
| (2,83) | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 3        | 0.23          |
| (2,83) | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 6        | 0.23          |
| (2,78) | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 7        | 0.23          |
| (2,75) | 1:34:E:LEU:O  | 1:32:D:ILE:H   | 1        | 0.23          |
| (2,73) | 1:32:D:ILE:O  | 1:34:E:LEU:H   | 7        | 0.23          |
| (2,72) | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 7        | 0.23          |
| (2,70) | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 5        | 0.23          |
| (2,69) | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 3        | 0.23          |
| (2,68) | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 2        | 0.23          |
| (2,67) | 1:34:C:LEU:O  | 1:32:B:ILE:H   | 9        | 0.23          |
| (2,65) | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 2        | 0.23          |
| (2,65) | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 4        | 0.23          |
| (2,64) | 1:31:H:ILE:O  | 1:35:G:MET:N   | 10       | 0.23          |
| (2,62) | 1:35:G:MET:O  | 1:31:H:ILE:N   | 2        | 0.23          |
| (2,62) | 1:35:G:MET:O  | 1:31:H:ILE:N   | 8        | 0.23          |
| (2,60) | 1:35:H:MET:O  | 1:31:G:ILE:N   | 7        | 0.23          |
| (2,60) | 1:35:H:MET:O  | 1:31:G:ILE:N   | 9        | 0.23          |
| (2,58) | 1:31:G:ILE:O  | 1:35:H:MET:N   | 7        | 0.23          |
| (2,58) | 1:31:G:ILE:O  | 1:35:H:MET:N   | 8        | 0.23          |
| (2,58) | 1:31:G:ILE:O  | 1:35:H:MET:N   | 9        | 0.23          |
| (2,52) | 1:35:F:MET:O  | 1:31:E:ILE:N   | 7        | 0.23          |
| (2,52) | 1:35:F:MET:O  | 1:31:E:ILE:N   | 9        | 0.23          |
| (2,42) | 1:31:C:ILE:O  | 1:35:D:MET:N   | 9        | 0.23          |
| (2,36) | 1:35:B:MET:O  | 1:31:A:ILE:N   | 2        | 0.23          |
| (2,34) | 1:31:A:ILE:O  | 1:35:B:MET:N   | 2        | 0.23          |
| (2,34) | 1:31:A:ILE:O  | 1:35:B:MET:N   | 5        | 0.23          |
| (2,32) | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 3        | 0.23          |
| (2,31) | 1:18:H:VAL:O  | 1:20:G:PHE:H   | 4        | 0.23          |
| (2,30) | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 6        | 0.23          |
| (2,29) | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 4        | 0.23          |
| (2,29) | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 10       | 0.23          |
| (2,27) | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 5        | 0.23          |
| (2,27) | 1:20:H:PHE:O  | 1:18:G:VAL:H   | 8        | 0.23          |
| (2,26) | 1:18:G:VAL:O  | 1:20:H:PHE:N   | 7        | 0.23          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,25)  | 1:18:G:VAL:O  | 1:20:H:PHE:H   | 2        | 0.23          |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 5        | 0.23          |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 7        | 0.23          |
| (2,23)  | 1:18:F:VAL:O  | 1:20:E:PHE:H   | 10       | 0.23          |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 9        | 0.23          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N   | 1        | 0.23          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N   | 3        | 0.23          |
| (2,17)  | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 10       | 0.23          |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 3        | 0.23          |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 8        | 0.23          |
| (2,13)  | 1:20:C:PHE:O  | 1:18:D:VAL:H   | 2        | 0.23          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N   | 8        | 0.23          |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H   | 9        | 0.23          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H   | 6        | 0.23          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H   | 9        | 0.23          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 10       | 0.23          |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 3        | 0.23          |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 9        | 0.23          |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 2        | 0.23          |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 5        | 0.23          |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N   | 6        | 0.23          |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 4        | 0.23          |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 10       | 0.23          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 1        | 0.23          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 2        | 0.23          |
| (1,95)  | 1:19:B:PHE:C  | 1:19:C:PHE:C   | 10       | 0.23          |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 2        | 0.23          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 4        | 0.23          |
| (1,31)  | 1:19:D:PHE:CZ | 1:34:D:LEU:CG  | 9        | 0.23          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 1        | 0.22          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 2        | 0.22          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 6        | 0.22          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 10       | 0.22          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 4        | 0.22          |
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 7        | 0.22          |
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 8        | 0.22          |
| (2,83)  | 1:34:G:LEU:O  | 1:32:F:ILE:H   | 10       | 0.22          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 4        | 0.22          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 3        | 0.22          |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 5        | 0.22          |
| (2,77)  | 1:34:D:LEU:O  | 1:32:E:ILE:H   | 1        | 0.22          |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 3        | 0.22          |

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| Key     | Atom-1        | Atom-2       | Model ID | Violation (Å) |
|---------|---------------|--------------|----------|---------------|
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N | 8        | 0.22          |
| (2,73)  | 1:32:D:ILE:O  | 1:34:E:LEU:H | 1        | 0.22          |
| (2,73)  | 1:32:D:ILE:O  | 1:34:E:LEU:H | 4        | 0.22          |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N | 6        | 0.22          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H | 8        | 0.22          |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N | 1        | 0.22          |
| (2,65)  | 1:32:B:ILE:O  | 1:34:C:LEU:H | 5        | 0.22          |
| (2,62)  | 1:35:G:MET:O  | 1:31:H:ILE:N | 4        | 0.22          |
| (2,62)  | 1:35:G:MET:O  | 1:31:H:ILE:N | 7        | 0.22          |
| (2,60)  | 1:35:H:MET:O  | 1:31:G:ILE:N | 3        | 0.22          |
| (2,60)  | 1:35:H:MET:O  | 1:31:G:ILE:N | 6        | 0.22          |
| (2,54)  | 1:35:E:MET:O  | 1:31:F:ILE:N | 1        | 0.22          |
| (2,50)  | 1:31:E:ILE:O  | 1:35:F:MET:N | 4        | 0.22          |
| (2,44)  | 1:35:D:MET:O  | 1:31:C:ILE:N | 9        | 0.22          |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N | 10       | 0.22          |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N | 1        | 0.22          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N | 6        | 0.22          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N | 8        | 0.22          |
| (2,31)  | 1:18:H:VAL:O  | 1:20:G:PHE:H | 2        | 0.22          |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N | 7        | 0.22          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N | 3        | 0.22          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N | 9        | 0.22          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N | 3        | 0.22          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N | 4        | 0.22          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N | 6        | 0.22          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N | 9        | 0.22          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N | 4        | 0.22          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N | 7        | 0.22          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N | 9        | 0.22          |
| (2,17)  | 1:18:E:VAL:O  | 1:20:F:PHE:H | 8        | 0.22          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N | 6        | 0.22          |
| (2,10)  | 1:18:C:VAL:O  | 1:20:D:PHE:N | 10       | 0.22          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N | 5        | 0.22          |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H | 2        | 0.22          |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H | 7        | 0.22          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N | 5        | 0.22          |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H | 4        | 0.22          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N | 10       | 0.22          |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H | 7        | 0.22          |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N | 9        | 0.22          |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N | 3        | 0.22          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N | 4        | 0.22          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 6        | 0.22          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 6        | 0.22          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 7        | 0.22          |
| (1,42)  | 1:21:F:ALA:CA | 1:32:F:ILE:CD1 | 5        | 0.22          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 8        | 0.22          |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 5        | 0.21          |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 9        | 0.21          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 2        | 0.21          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 7        | 0.21          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 5        | 0.21          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 10       | 0.21          |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 4        | 0.21          |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 10       | 0.21          |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 6        | 0.21          |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 10       | 0.21          |
| (2,73)  | 1:32:D:ILE:O  | 1:34:E:LEU:H   | 6        | 0.21          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 5        | 0.21          |
| (2,69)  | 1:34:B:LEU:O  | 1:32:C:ILE:H   | 1        | 0.21          |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 4        | 0.21          |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 6        | 0.21          |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 7        | 0.21          |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 9        | 0.21          |
| (2,65)  | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 3        | 0.21          |
| (2,65)  | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 7        | 0.21          |
| (2,65)  | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 9        | 0.21          |
| (2,65)  | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 10       | 0.21          |
| (2,58)  | 1:31:G:ILE:O  | 1:35:H:MET:N   | 6        | 0.21          |
| (2,52)  | 1:35:F:MET:O  | 1:31:E:ILE:N   | 2        | 0.21          |
| (2,41)  | 1:31:C:ILE:O  | 1:35:D:MET:H   | 2        | 0.21          |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 1        | 0.21          |
| (2,34)  | 1:31:A:ILE:O  | 1:35:B:MET:N   | 9        | 0.21          |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 4        | 0.21          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 7        | 0.21          |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 5        | 0.21          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 2        | 0.21          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 6        | 0.21          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 10       | 0.21          |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 6        | 0.21          |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 8        | 0.21          |
| (2,19)  | 1:20:F:PHE:O  | 1:18:E:VAL:H   | 5        | 0.21          |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 6        | 0.21          |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 9        | 0.21          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 10       | 0.21          |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H   | 8        | 0.21          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 10       | 0.21          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H   | 2        | 0.21          |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H   | 7        | 0.21          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 7        | 0.21          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 5        | 0.21          |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 3        | 0.21          |
| (1,123) | 1:21:B:ALA:CB | 1:17:A:LEU:N   | 1        | 0.21          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 9        | 0.21          |
| (1,39)  | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 9        | 0.21          |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 8        | 0.21          |
| (1,23)  | 1:19:C:PHE:CZ | 1:34:C:LEU:CG  | 10       | 0.21          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 9        | 0.2           |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 2        | 0.2           |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 6        | 0.2           |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 3        | 0.2           |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 10       | 0.2           |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 4        | 0.2           |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 6        | 0.2           |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 9        | 0.2           |
| (2,76)  | 1:34:E:LEU:O  | 1:32:D:ILE:N   | 1        | 0.2           |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 2        | 0.2           |
| (2,72)  | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 8        | 0.2           |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 8        | 0.2           |
| (2,68)  | 1:34:C:LEU:O  | 1:32:B:ILE:N   | 10       | 0.2           |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 2        | 0.2           |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 5        | 0.2           |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 8        | 0.2           |
| (2,60)  | 1:35:H:MET:O  | 1:31:G:ILE:N   | 4        | 0.2           |
| (2,31)  | 1:18:H:VAL:O  | 1:20:G:PHE:H   | 10       | 0.2           |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 2        | 0.2           |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 4        | 0.2           |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 10       | 0.2           |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 1        | 0.2           |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N   | 8        | 0.2           |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 2        | 0.2           |
| (2,22)  | 1:20:E:PHE:O  | 1:18:F:VAL:N   | 2        | 0.2           |
| (2,17)  | 1:18:E:VAL:O  | 1:20:F:PHE:H   | 5        | 0.2           |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 2        | 0.2           |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 3        | 0.2           |
| (2,5)   | 1:20:A:PHE:O  | 1:18:B:VAL:H   | 8        | 0.2           |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 9        | 0.2           |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 2        | 0.2           |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 7        | 0.2           |
| (1,64)  | 1:21:H:ALA:CA | 1:32:H:ILE:CG1 | 5        | 0.2           |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 3        | 0.2           |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 6        | 0.2           |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 8        | 0.2           |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 9        | 0.2           |
| (2,85)  | 1:34:F:LEU:O  | 1:32:G:ILE:H   | 7        | 0.19          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 2        | 0.19          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 5        | 0.19          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 6        | 0.19          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 9        | 0.19          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 9        | 0.19          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 10       | 0.19          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 1        | 0.19          |
| (2,78)  | 1:34:D:LEU:O  | 1:32:E:ILE:N   | 1        | 0.19          |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 3        | 0.19          |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 5        | 0.19          |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 6        | 0.19          |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 7        | 0.19          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 1        | 0.19          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 6        | 0.19          |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 3        | 0.19          |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 9        | 0.19          |
| (2,62)  | 1:35:G:MET:O  | 1:31:H:ILE:N   | 6        | 0.19          |
| (2,58)  | 1:31:G:ILE:O  | 1:35:H:MET:N   | 4        | 0.19          |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 10       | 0.19          |
| (2,38)  | 1:35:A:MET:O  | 1:31:B:ILE:N   | 5        | 0.19          |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N   | 10       | 0.19          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 4        | 0.19          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 8        | 0.19          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N   | 2        | 0.19          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N   | 10       | 0.19          |
| (2,24)  | 1:18:F:VAL:O  | 1:20:E:PHE:N   | 10       | 0.19          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N   | 10       | 0.19          |
| (2,16)  | 1:18:D:VAL:O  | 1:20:C:PHE:N   | 10       | 0.19          |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 10       | 0.19          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 4        | 0.19          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 2        | 0.19          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 3        | 0.19          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 4        | 0.19          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 6        | 0.19          |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 4        | 0.19          |
| (1,125) | 1:21:D:ALA:CB | 1:17:C:LEU:N   | 1        | 0.19          |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 3        | 0.19          |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 6        | 0.19          |
| (1,55)  | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 4        | 0.19          |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 1        | 0.19          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 3        | 0.19          |
| (1,8)   | 1:21:A:ALA:CA | 1:32:A:ILE:CG1 | 8        | 0.19          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 6        | 0.18          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 7        | 0.18          |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 8        | 0.18          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 5        | 0.18          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 9        | 0.18          |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 1        | 0.18          |
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 9        | 0.18          |
| (2,72)  | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 5        | 0.18          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 10       | 0.18          |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 4        | 0.18          |
| (2,65)  | 1:32:B:ILE:O  | 1:34:C:LEU:H   | 6        | 0.18          |
| (2,40)  | 1:31:B:ILE:O  | 1:35:A:MET:N   | 5        | 0.18          |
| (2,36)  | 1:35:B:MET:O  | 1:31:A:ILE:N   | 5        | 0.18          |
| (2,33)  | 1:31:A:ILE:O  | 1:35:B:MET:H   | 7        | 0.18          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 2        | 0.18          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 10       | 0.18          |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 5        | 0.18          |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 6        | 0.18          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N   | 6        | 0.18          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 3        | 0.18          |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N   | 4        | 0.18          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 5        | 0.18          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 9        | 0.18          |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 1        | 0.18          |
| (1,50)  | 1:21:G:ALA:CA | 1:32:G:ILE:CD1 | 4        | 0.18          |
| (1,47)  | 1:19:F:PHE:CZ | 1:34:F:LEU:CG  | 6        | 0.18          |
| (1,40)  | 1:21:E:ALA:CA | 1:32:E:ILE:CG1 | 7        | 0.18          |
| (1,39)  | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 4        | 0.18          |
| (1,39)  | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 7        | 0.18          |
| (1,17)  | 1:19:C:PHE:CZ | 1:32:C:ILE:CD1 | 1        | 0.18          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 2        | 0.17          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 8        | 0.17          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 10       | 0.17          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 10       | 0.17          |
| (2,79)  | 1:32:E:ILE:O  | 1:34:D:LEU:H   | 4        | 0.17          |
| (2,71)  | 1:32:C:ILE:O  | 1:34:B:LEU:H   | 3        | 0.17          |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 1        | 0.17          |
| (2,70)  | 1:34:B:LEU:O  | 1:32:C:ILE:N   | 10       | 0.17          |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 3        | 0.17          |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 7        | 0.17          |
| (2,29)  | 1:20:G:PHE:O  | 1:18:H:VAL:H   | 1        | 0.17          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N   | 1        | 0.17          |
| (2,20)  | 1:20:F:PHE:O  | 1:18:E:VAL:N   | 1        | 0.17          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N   | 8        | 0.17          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 4        | 0.17          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 7        | 0.17          |
| (2,7)   | 1:18:B:VAL:O  | 1:20:A:PHE:H   | 1        | 0.17          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 1        | 0.17          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 7        | 0.17          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 9        | 0.17          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 3        | 0.17          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 7        | 0.17          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 8        | 0.17          |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 1        | 0.17          |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 9        | 0.17          |
| (1,117) | 1:21:B:ALA:CB | 1:17:C:LEU:N   | 10       | 0.17          |
| (1,101) | 1:33:G:GLY:C  | 1:33:H:GLY:C   | 3        | 0.17          |
| (1,101) | 1:33:G:GLY:C  | 1:33:H:GLY:C   | 4        | 0.17          |
| (1,101) | 1:33:G:GLY:C  | 1:33:H:GLY:C   | 7        | 0.17          |
| (1,98)  | 1:33:A:GLY:C  | 1:33:B:GLY:C   | 5        | 0.17          |
| (1,47)  | 1:19:F:PHE:CZ | 1:34:F:LEU:CG  | 3        | 0.17          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 5        | 0.17          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 6        | 0.17          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 10       | 0.17          |
| (1,8)   | 1:21:A:ALA:CA | 1:32:A:ILE:CG1 | 1        | 0.17          |
| (1,8)   | 1:21:A:ALA:CA | 1:32:A:ILE:CG1 | 5        | 0.17          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 9        | 0.16          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 10       | 0.16          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 8        | 0.16          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 3        | 0.16          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 2        | 0.16          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 6        | 0.16          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 3        | 0.16          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 7        | 0.16          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 1        | 0.16          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,74)  | 1:32:D:ILE:O  | 1:34:E:LEU:N   | 4        | 0.16          |
| (2,72)  | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 6        | 0.16          |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 10       | 0.16          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 5        | 0.16          |
| (2,31)  | 1:18:H:VAL:O  | 1:20:G:PHE:H   | 1        | 0.16          |
| (2,18)  | 1:18:E:VAL:O  | 1:20:F:PHE:N   | 5        | 0.16          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 9        | 0.16          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 9        | 0.16          |
| (2,3)   | 1:20:B:PHE:O  | 1:18:A:VAL:H   | 1        | 0.16          |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 9        | 0.16          |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 3        | 0.16          |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 5        | 0.16          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 10       | 0.16          |
| (1,119) | 1:21:D:ALA:CB | 1:17:E:LEU:N   | 10       | 0.16          |
| (1,64)  | 1:21:H:ALA:CA | 1:32:H:ILE:CG1 | 2        | 0.16          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 2        | 0.16          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 5        | 0.15          |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 3        | 0.15          |
| (2,86)  | 1:34:F:LEU:O  | 1:32:G:ILE:N   | 7        | 0.15          |
| (2,84)  | 1:34:G:LEU:O  | 1:32:F:ILE:N   | 7        | 0.15          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 9        | 0.15          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 8        | 0.15          |
| (2,72)  | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 1        | 0.15          |
| (2,72)  | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 3        | 0.15          |
| (2,66)  | 1:32:B:ILE:O  | 1:34:C:LEU:N   | 6        | 0.15          |
| (2,42)  | 1:31:C:ILE:O  | 1:35:D:MET:N   | 2        | 0.15          |
| (2,34)  | 1:31:A:ILE:O  | 1:35:B:MET:N   | 4        | 0.15          |
| (2,30)  | 1:20:G:PHE:O  | 1:18:H:VAL:N   | 1        | 0.15          |
| (2,28)  | 1:20:H:PHE:O  | 1:18:G:VAL:N   | 5        | 0.15          |
| (2,26)  | 1:18:G:VAL:O  | 1:20:H:PHE:N   | 5        | 0.15          |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 9        | 0.15          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 6        | 0.15          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 6        | 0.15          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 2        | 0.15          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 4        | 0.15          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 6        | 0.15          |
| (1,124) | 1:21:C:ALA:CB | 1:17:B:LEU:N   | 6        | 0.15          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 8        | 0.15          |
| (1,120) | 1:21:E:ALA:CB | 1:17:F:LEU:N   | 6        | 0.15          |
| (1,101) | 1:33:G:GLY:C  | 1:33:H:GLY:C   | 6        | 0.15          |
| (1,57)  | 1:19:H:PHE:CZ | 1:32:H:ILE:CD1 | 1        | 0.15          |
| (1,55)  | 1:19:G:PHE:CZ | 1:34:G:LEU:CG  | 10       | 0.15          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 1        | 0.15          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 3        | 0.15          |
| (1,48)  | 1:21:F:ALA:CA | 1:32:F:ILE:CG1 | 6        | 0.15          |
| (1,31)  | 1:19:D:PHE:CZ | 1:34:D:LEU:CG  | 4        | 0.15          |
| (1,7)   | 1:19:A:PHE:CZ | 1:34:A:LEU:CG  | 6        | 0.15          |
| (2,87)  | 1:32:G:ILE:O  | 1:34:F:LEU:H   | 3        | 0.14          |
| (2,80)  | 1:32:E:ILE:O  | 1:34:D:LEU:N   | 4        | 0.14          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 2        | 0.14          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 8        | 0.14          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 2        | 0.14          |
| (2,6)   | 1:20:A:PHE:O  | 1:18:B:VAL:N   | 8        | 0.14          |
| (2,2)   | 1:18:A:VAL:O  | 1:20:B:PHE:N   | 9        | 0.14          |
| (1,64)  | 1:21:H:ALA:CA | 1:32:H:ILE:CG1 | 4        | 0.14          |
| (1,60)  | 1:19:H:PHE:CZ | 1:32:H:ILE:CG2 | 6        | 0.14          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 7        | 0.14          |
| (1,16)  | 1:21:B:ALA:CA | 1:32:B:ILE:CG1 | 9        | 0.14          |
| (1,15)  | 1:19:B:PHE:CZ | 1:34:B:LEU:CG  | 6        | 0.14          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 7        | 0.13          |
| (2,81)  | 1:32:F:ILE:O  | 1:34:G:LEU:H   | 5        | 0.13          |
| (2,72)  | 1:32:C:ILE:O  | 1:34:B:LEU:N   | 10       | 0.13          |
| (2,32)  | 1:18:H:VAL:O  | 1:20:G:PHE:N   | 1        | 0.13          |
| (2,4)   | 1:20:B:PHE:O  | 1:18:A:VAL:N   | 1        | 0.13          |
| (1,128) | 1:21:G:ALA:CB | 1:17:F:LEU:N   | 7        | 0.13          |
| (1,122) | 1:21:G:ALA:CB | 1:17:H:LEU:N   | 2        | 0.13          |
| (1,121) | 1:21:F:ALA:CB | 1:17:G:LEU:N   | 5        | 0.13          |
| (1,118) | 1:21:C:ALA:CB | 1:17:D:LEU:N   | 4        | 0.13          |
| (1,58)  | 1:21:H:ALA:CA | 1:32:H:ILE:CD1 | 4        | 0.13          |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 4        | 0.13          |
| (1,39)  | 1:19:E:PHE:CZ | 1:34:E:LEU:CG  | 10       | 0.13          |
| (1,32)  | 1:21:D:ALA:CA | 1:32:D:ILE:CG1 | 4        | 0.13          |
| (1,24)  | 1:21:C:ALA:CA | 1:32:C:ILE:CG1 | 10       | 0.13          |
| (1,15)  | 1:19:B:PHE:CZ | 1:34:B:LEU:CG  | 8        | 0.13          |
| (1,4)   | 1:19:A:PHE:CZ | 1:32:A:ILE:CG2 | 5        | 0.13          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 8        | 0.12          |
| (2,34)  | 1:31:A:ILE:O  | 1:35:B:MET:N   | 7        | 0.12          |
| (2,14)  | 1:20:C:PHE:O  | 1:18:D:VAL:N   | 2        | 0.12          |
| (1,123) | 1:21:B:ALA:CB | 1:17:A:LEU:N   | 5        | 0.12          |
| (1,105) | 1:30:D:ALA:CB | 1:36:E:VAL:N   | 6        | 0.12          |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 7        | 0.12          |
| (1,8)   | 1:21:A:ALA:CA | 1:32:A:ILE:CG1 | 4        | 0.12          |
| (1,8)   | 1:21:A:ALA:CA | 1:32:A:ILE:CG1 | 10       | 0.12          |
| (1,1)   | 1:19:A:PHE:CZ | 1:32:A:ILE:CD1 | 4        | 0.12          |

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| Key     | Atom-1        | Atom-2         | Model ID | Violation (Å) |
|---------|---------------|----------------|----------|---------------|
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 5        | 0.11          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 3        | 0.11          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 5        | 0.11          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 7        | 0.11          |
| (2,82)  | 1:32:F:ILE:O  | 1:34:G:LEU:N   | 8        | 0.11          |
| (2,8)   | 1:18:B:VAL:O  | 1:20:A:PHE:N   | 1        | 0.11          |
| (1,126) | 1:21:E:ALA:CB | 1:17:D:LEU:N   | 4        | 0.11          |
| (1,116) | 1:21:A:ALA:CB | 1:17:B:LEU:N   | 1        | 0.11          |
| (1,101) | 1:33:G:GLY:C  | 1:33:H:GLY:C   | 2        | 0.11          |
| (1,60)  | 1:19:H:PHE:CZ | 1:32:H:ILE:CG2 | 3        | 0.11          |
| (1,1)   | 1:19:A:PHE:CZ | 1:32:A:ILE:CD1 | 2        | 0.11          |
| (2,88)  | 1:32:G:ILE:O  | 1:34:F:LEU:N   | 3        | 0.1           |
| (2,1)   | 1:18:A:VAL:O  | 1:20:B:PHE:H   | 1        | 0.1           |
| (1,107) | 1:30:F:ALA:CB | 1:36:G:VAL:N   | 4        | 0.1           |
| (1,56)  | 1:21:G:ALA:CA | 1:32:G:ILE:CG1 | 8        | 0.1           |
| (1,47)  | 1:19:F:PHE:CZ | 1:34:F:LEU:CG  | 1        | 0.1           |

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

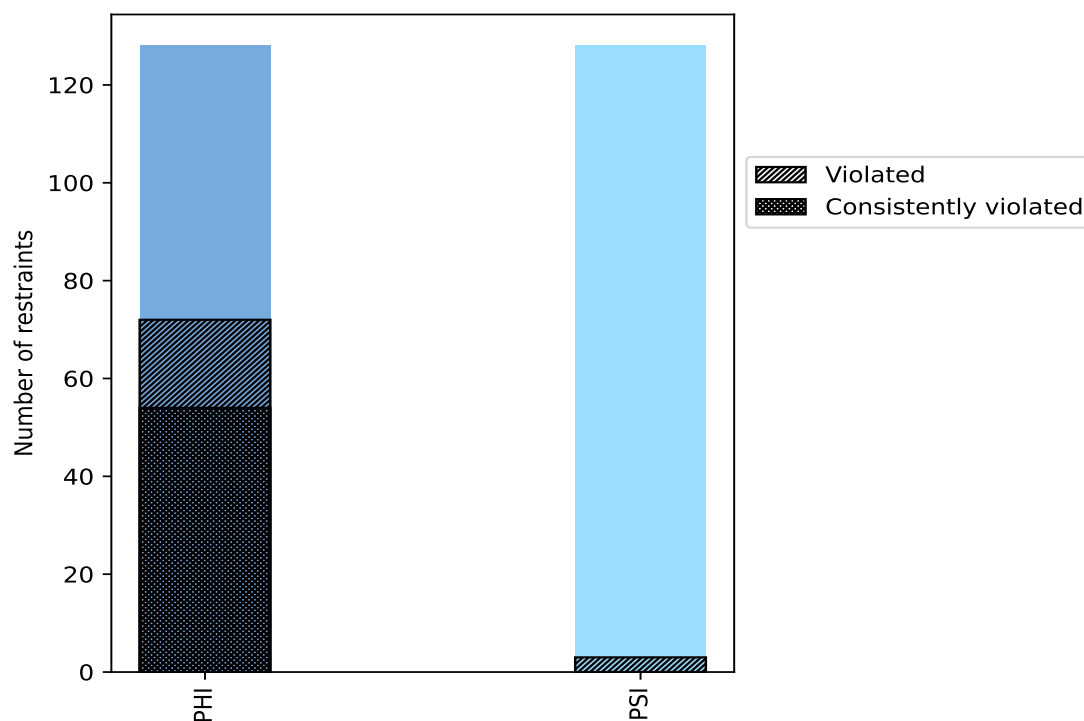
### 10.1 Summary of dihedral-angle violations [i](#)

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> |
| PHI        | 128   | 50.0           | 72                    | 56.2           | 28.1           | 54                                 | 42.2           | 21.1           |
| PSI        | 128   | 50.0           | 3                     | 2.3            | 1.2            | 0                                  | 0.0            | 0.0            |
| Total      | 256   | 100.0          | 75                    | 29.3           | 29.3           | 54                                 | 21.1           | 21.1           |

<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

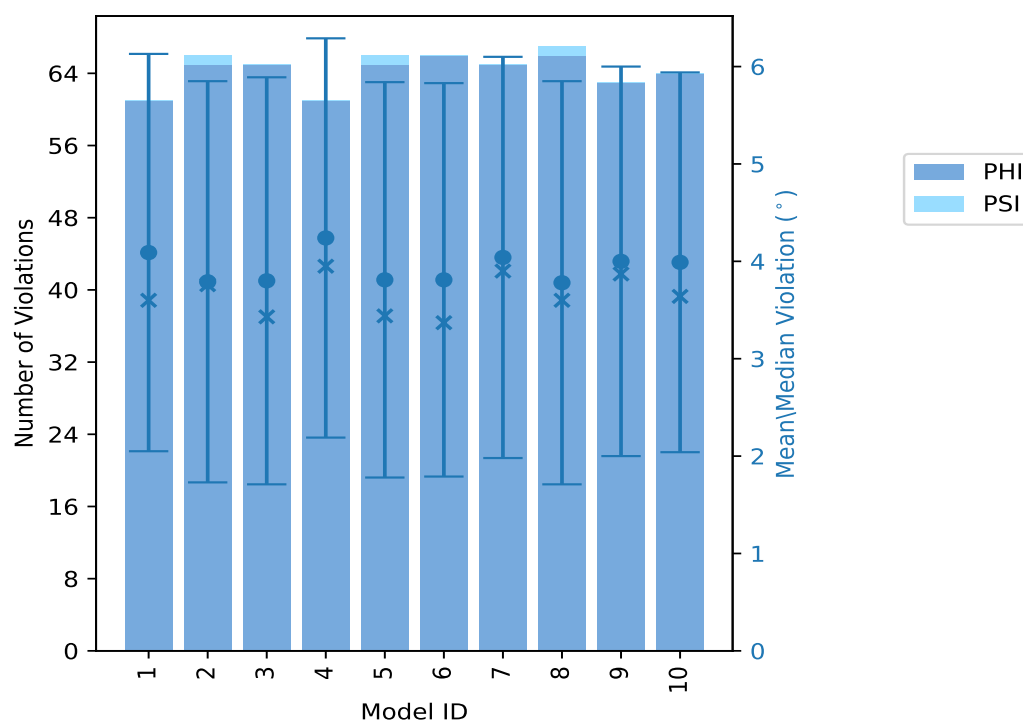


## 10.2 Dihedral-angle violation statistics for each model [i](#)

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PHI                  | PSI | Total |          |         |        |            |
| 1        | 61                   | 0   | 61    | 4.09     | 8.27    | 2.04   | 3.6        |
| 2        | 65                   | 1   | 66    | 3.79     | 8.34    | 2.06   | 3.76       |
| 3        | 65                   | 0   | 65    | 3.8      | 8.31    | 2.09   | 3.43       |
| 4        | 61                   | 0   | 61    | 4.24     | 8.51    | 2.05   | 3.95       |
| 5        | 65                   | 1   | 66    | 3.81     | 8.36    | 2.03   | 3.44       |
| 6        | 66                   | 0   | 66    | 3.81     | 8.07    | 2.02   | 3.37       |
| 7        | 65                   | 0   | 65    | 4.04     | 8.53    | 2.06   | 3.9        |
| 8        | 66                   | 1   | 67    | 3.78     | 8.36    | 2.07   | 3.6        |
| 9        | 63                   | 0   | 63    | 4.0      | 8.47    | 2.0    | 3.87       |
| 10       | 64                   | 0   | 64    | 3.99     | 8.34    | 1.95   | 3.64       |

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



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

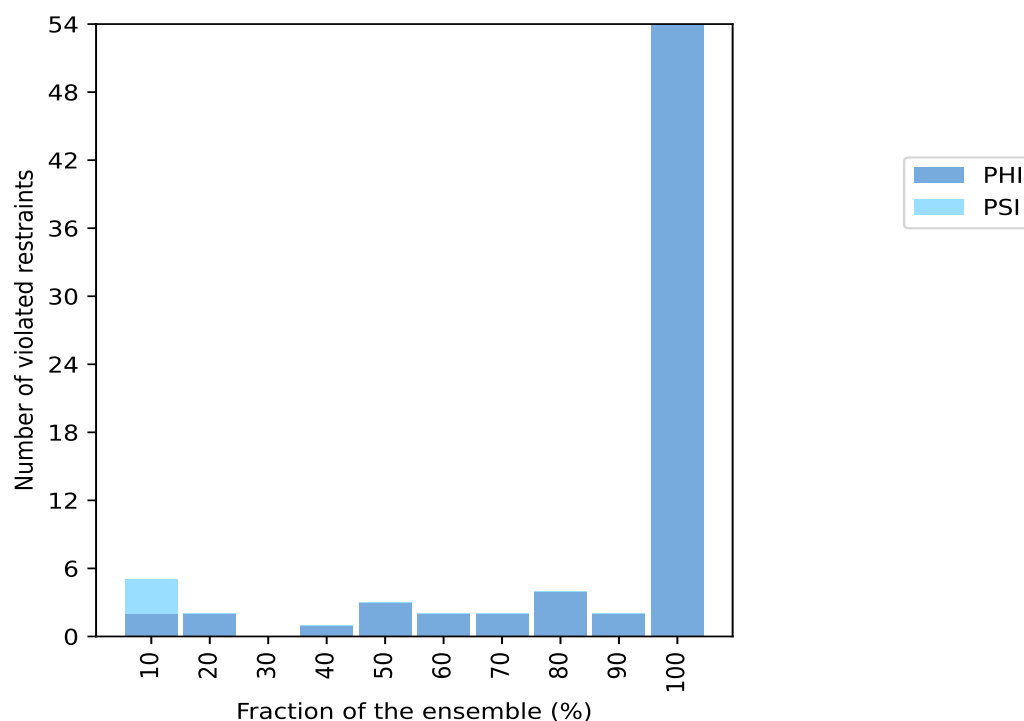
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PHI                           | PSI | Total | Count <sup>1</sup>       | %     |
| 2                             | 3   | 5     | 1                        | 10.0  |
| 2                             | 0   | 2     | 2                        | 20.0  |
| 0                             | 0   | 0     | 3                        | 30.0  |
| 1                             | 0   | 1     | 4                        | 40.0  |
| 3                             | 0   | 3     | 5                        | 50.0  |
| 2                             | 0   | 2     | 6                        | 60.0  |
| 2                             | 0   | 2     | 7                        | 70.0  |
| 4                             | 0   | 4     | 8                        | 80.0  |
| 2                             | 0   | 2     | 9                        | 90.0  |
| 54                            | 0   | 54    | 10                       | 100.0 |

<sup>1</sup> Number of models with violations

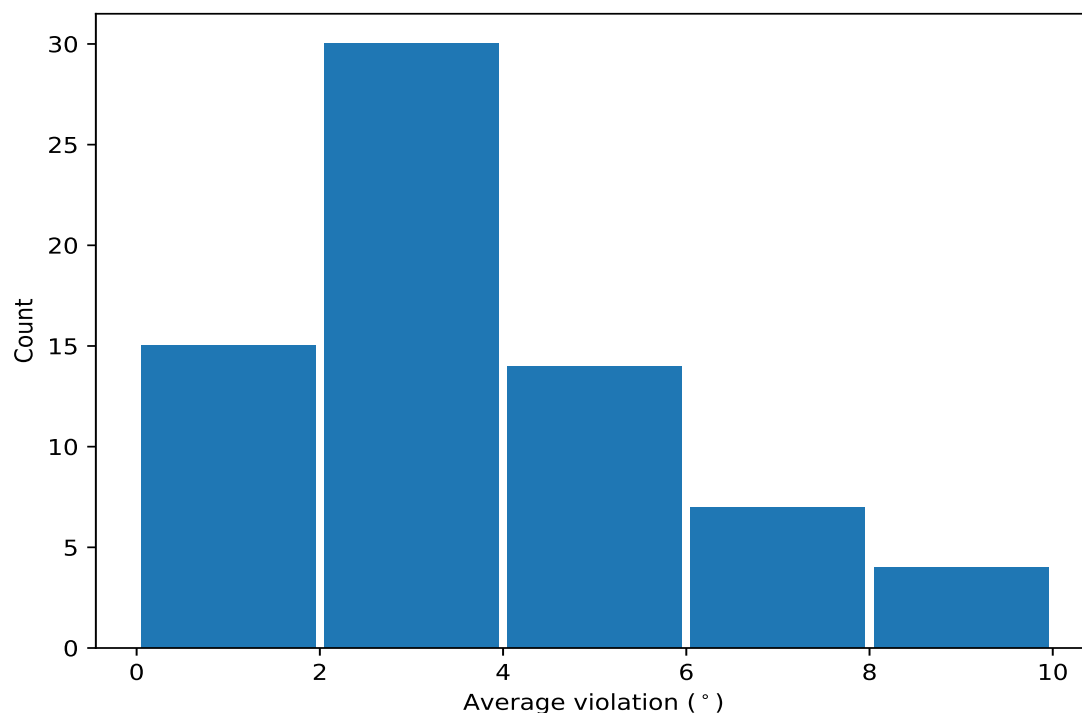
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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

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

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



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

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

| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|--------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 10                  | 8.27 | 0.18            | 8.28   |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 10                  | 8.2  | 0.2             | 8.2    |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 10                  | 8.02 | 0.2             | 7.92   |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 10                  | 8.0  | 0.21            | 7.94   |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 10                  | 7.95 | 0.3             | 7.96   |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 10                  | 7.93 | 0.2             | 7.87   |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 10                  | 7.9  | 0.23            | 7.99   |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 10                  | 7.83 | 0.31            | 7.89   |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 10                  | 6.37 | 0.6             | 6.16   |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 10                  | 6.08 | 0.58            | 6.13   |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 10                  | 6.01 | 0.91            | 5.93   |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 10                  | 5.78 | 0.69            | 5.56   |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 10                  | 5.25 | 0.99            | 5.48   |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|--------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 10                  | 5.24 | 0.43            | 5.34   |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 10                  | 4.74 | 0.25            | 4.82   |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 10                  | 4.65 | 0.45            | 4.65   |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 10                  | 4.65 | 0.69            | 4.74   |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 10                  | 4.54 | 1.13            | 4.98   |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 10                  | 4.54 | 0.34            | 4.52   |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 10                  | 4.54 | 0.52            | 4.63   |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 10                  | 4.45 | 0.58            | 4.54   |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 10                  | 4.36 | 0.17            | 4.42   |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 10                  | 4.32 | 0.21            | 4.31   |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 10                  | 4.23 | 0.6             | 4.28   |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 10                  | 4.13 | 0.49            | 4.04   |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 10                  | 3.97 | 0.42            | 4.01   |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 10                  | 3.96 | 0.39            | 3.94   |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 10                  | 3.92 | 0.35            | 4.03   |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 10                  | 3.9  | 0.45            | 3.76   |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 10                  | 3.86 | 0.37            | 3.94   |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 10                  | 3.82 | 0.2             | 3.81   |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 10                  | 3.69 | 0.23            | 3.66   |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 10                  | 3.68 | 0.59            | 3.76   |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 10                  | 3.61 | 1.28            | 4.11   |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 10                  | 3.61 | 0.54            | 3.59   |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 10                  | 3.49 | 0.28            | 3.43   |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 10                  | 3.48 | 0.39            | 3.4    |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 10                  | 2.92 | 0.37            | 2.98   |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 10                  | 2.92 | 0.3             | 2.96   |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 10                  | 2.88 | 0.39            | 2.88   |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 10                  | 2.87 | 0.41            | 2.9    |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 10                  | 2.76 | 0.45            | 2.81   |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 10                  | 2.74 | 0.56            | 2.66   |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N | 1:32:F:ILE:CA | 1:32:F:ILE:C | 10                  | 2.36 | 1.31            | 1.73   |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 10                  | 2.24 | 0.92            | 1.97   |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 10                  | 2.22 | 0.47            | 2.27   |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N | 1:32:C:ILE:CA | 1:32:C:ILE:C | 10                  | 2.19 | 0.96            | 1.82   |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 10                  | 2.12 | 0.5             | 2.29   |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 10                  | 2.1  | 0.53            | 2.06   |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N | 1:18:H:VAL:CA | 1:18:H:VAL:C | 10                  | 1.97 | 0.47            | 1.9    |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N | 1:32:G:ILE:CA | 1:32:G:ILE:C | 10                  | 1.96 | 0.88            | 1.6    |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N | 1:34:H:LEU:CA | 1:34:H:LEU:C | 10                  | 1.89 | 0.55            | 2.04   |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N | 1:32:D:ILE:CA | 1:32:D:ILE:C | 10                  | 1.86 | 0.74            | 1.85   |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 10                  | 1.75 | 0.24            | 1.78   |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 9                   | 2.24 | 0.93            | 1.98   |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N | 1:34:E:LEU:CA | 1:34:E:LEU:C | 9                   | 2.2  | 0.6             | 2.42   |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 8                   | 3.3  | 0.89            | 3.72   |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 8                   | 2.17 | 0.32            | 2.14   |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N | 1:34:A:LEU:CA | 1:34:A:LEU:C | 8                   | 1.7  | 0.61            | 1.63   |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N | 1:18:G:VAL:CA | 1:18:G:VAL:C | 8                   | 1.66 | 0.33            | 1.67   |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 7                   | 2.11 | 0.25            | 2.12   |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N | 1:18:E:VAL:CA | 1:18:E:VAL:C | 7                   | 1.76 | 0.17            | 1.7    |
| (1,109) | 1:33:G:GLY:C | 1:34:G:LEU:N | 1:34:G:LEU:CA | 1:34:G:LEU:C | 6                   | 2.11 | 0.87            | 1.7    |
| (1,94)  | 1:34:F:LEU:C | 1:35:F:MET:N | 1:35:F:MET:CA | 1:35:F:MET:C | 6                   | 1.58 | 0.37            | 1.58   |

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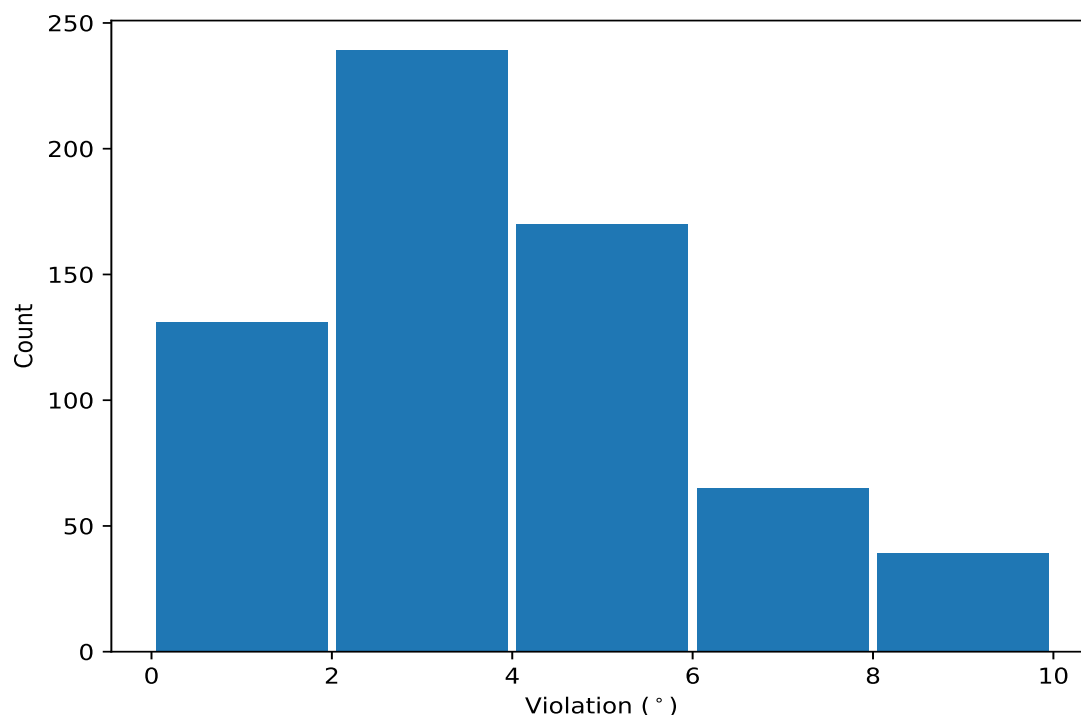
| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Models <sup>1</sup> | Mean | SD <sup>2</sup> | Median |
|---------|--------------|--------------|---------------|--------------|---------------------|------|-----------------|--------|
| (1,110) | 1:34:G:LEU:C | 1:35:G:MET:N | 1:35:G:MET:CA | 1:35:G:MET:C | 5                   | 1.86 | 0.43            | 2.04   |
| (1,35)  | 1:17:C:LEU:C | 1:18:C:VAL:N | 1:18:C:VAL:CA | 1:18:C:VAL:C | 5                   | 1.76 | 0.38            | 1.92   |
| (1,46)  | 1:34:C:LEU:C | 1:35:C:MET:N | 1:35:C:MET:CA | 1:35:C:MET:C | 5                   | 1.45 | 0.24            | 1.37   |
| (1,30)  | 1:34:B:LEU:C | 1:35:B:MET:N | 1:35:B:MET:CA | 1:35:B:MET:C | 4                   | 1.53 | 0.42            | 1.35   |
| (1,78)  | 1:34:E:LEU:C | 1:35:E:MET:N | 1:35:E:MET:CA | 1:35:E:MET:C | 2                   | 1.58 | 0.16            | 1.58   |
| (1,62)  | 1:34:D:LEU:C | 1:35:D:MET:N | 1:35:D:MET:CA | 1:35:D:MET:C | 2                   | 1.4  | 0.28            | 1.4    |

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

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

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

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



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

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

| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 7        | 8.53          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 4        | 8.51          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 9        | 8.47          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 7        | 8.46          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 9        | 8.41          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 8        | 8.36          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 4        | 8.36          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 8        | 8.36          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 5        | 8.36          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 2        | 8.34          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 10       | 8.34          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 9        | 8.34          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 5        | 8.34          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 3        | 8.31          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 1        | 8.27          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 7        | 8.26          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 2        | 8.25          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 1        | 8.24          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 1        | 8.23          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 1        | 8.21          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 10       | 8.21          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 3        | 8.2           |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 3        | 8.18          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 4        | 8.18          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 4        | 8.17          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 3        | 8.16          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 9        | 8.15          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 10       | 8.15          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 2        | 8.14          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 6        | 8.07          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 4        | 8.07          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 10       | 8.05          |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 6        | 8.05          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 8        | 8.03          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 7        | 8.03          |
| (1,114) | 1:16:H:LYS:C | 1:17:H:LEU:N | 1:17:H:LEU:CA | 1:17:H:LEU:C | 5        | 8.02          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 1        | 8.02          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 2        | 8.01          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 4        | 8.01          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 5        | 7.99          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 6        | 7.99          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 4        | 7.99          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 10       | 7.98          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 9        | 7.98          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 6        | 7.97          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 3        | 7.96          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 1        | 7.95          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 9        | 7.95          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 1        | 7.94          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 6        | 7.93          |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 4        | 7.93          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 2        | 7.92          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 5        | 7.92          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 8        | 7.92          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 7        | 7.9           |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 10       | 7.9           |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 2        | 7.89          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 9        | 7.89          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 1        | 7.89          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 7        | 7.89          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 5        | 7.87          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 3        | 7.87          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 8        | 7.87          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 9        | 7.87          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 7        | 7.87          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 4        | 7.86          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 3        | 7.86          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 8        | 7.84          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 8        | 7.82          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 7        | 7.8           |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 6        | 7.8           |
| (1,18)  | 1:16:B:LYS:C | 1:17:B:LEU:N | 1:17:B:LEU:CA | 1:17:B:LEU:C | 5        | 7.79          |
| (1,50)  | 1:16:D:LYS:C | 1:17:D:LEU:N | 1:17:D:LEU:CA | 1:17:D:LEU:C | 6        | 7.76          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 2        | 7.75          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 6        | 7.75          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 3        | 7.74          |
| (1,34)  | 1:16:C:LYS:C | 1:17:C:LEU:N | 1:17:C:LEU:CA | 1:17:C:LEU:C | 10       | 7.71          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 7        | 7.68          |
| (1,2)   | 1:16:A:LYS:C | 1:17:A:LEU:N | 1:17:A:LEU:CA | 1:17:A:LEU:C | 2        | 7.65          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 1        | 7.27          |
| (1,98)  | 1:16:G:LYS:C | 1:17:G:LEU:N | 1:17:G:LEU:CA | 1:17:G:LEU:C | 5        | 7.24          |
| (1,82)  | 1:16:F:LYS:C | 1:17:F:LEU:N | 1:17:F:LEU:CA | 1:17:F:LEU:C | 10       | 7.24          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 1        | 7.08          |
| (1,66)  | 1:16:E:LYS:C | 1:17:E:LEU:N | 1:17:E:LEU:CA | 1:17:E:LEU:C | 8        | 6.98          |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 3        | 6.78          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 5        | 6.7           |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 4        | 6.63          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 4        | 6.5           |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 8        | 6.5           |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 10       | 6.46          |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 1        | 6.46          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 9        | 6.4           |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 6        | 6.25          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 5        | 6.22          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 10       | 6.16          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 7        | 6.14          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 6        | 6.12          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 2        | 6.09          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 6        | 6.09          |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 7        | 6.08          |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 2        | 6.07          |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 9        | 6.05          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 4        | 6.01          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 5        | 6.01          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 3        | 5.98          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 3        | 5.97          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 5        | 5.89          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 8        | 5.84          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 2        | 5.81          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 8        | 5.75          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 3        | 5.72          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 2        | 5.72          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 4        | 5.69          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 9        | 5.65          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 4        | 5.65          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 8        | 5.65          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 9        | 5.61          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 7        | 5.61          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 8        | 5.6           |
| (1,20)  | 1:18:B:VAL:C | 1:19:B:PHE:N | 1:19:B:PHE:CA | 1:19:B:PHE:C | 10       | 5.6           |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 8        | 5.53          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 7        | 5.52          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 10       | 5.52          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 6        | 5.49          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 7        | 5.47          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 8        | 5.46          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 6        | 5.45          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 6        | 5.45          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 2        | 5.44          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 9        | 5.39          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 5        | 5.36          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 3        | 5.36          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 4        | 5.33          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 10       | 5.31          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 4        | 5.31          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 6        | 5.28          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 10       | 5.26          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 10       | 5.25          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 7        | 5.25          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 9        | 5.18          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 7        | 5.17          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 3        | 5.11          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 3        | 5.11          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 6        | 5.08          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 8        | 5.08          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 5        | 5.07          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 5        | 5.06          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 1        | 5.05          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 6        | 5.04          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 4        | 5.02          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 5        | 4.99          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 6        | 4.97          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 3        | 4.92          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 2        | 4.92          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 1        | 4.92          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 5        | 4.9           |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 1        | 4.89          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 7        | 4.89          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 7        | 4.89          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 8        | 4.87          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 8        | 4.85          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 3        | 4.85          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 1        | 4.85          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 1        | 4.84          |
| (1,52)  | 1:18:D:VAL:C | 1:19:D:PHE:N | 1:19:D:PHE:CA | 1:19:D:PHE:C | 1        | 4.84          |
| (1,100) | 1:18:G:VAL:C | 1:19:G:PHE:N | 1:19:G:PHE:CA | 1:19:G:PHE:C | 2        | 4.83          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 10       | 4.83          |
| (1,68)  | 1:18:E:VAL:C | 1:19:E:PHE:N | 1:19:E:PHE:CA | 1:19:E:PHE:C | 2        | 4.82          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 7        | 4.82          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 1        | 4.79          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 10       | 4.79          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 7        | 4.79          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 8        | 4.78          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 6        | 4.77          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 6        | 4.77          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 4        | 4.75          |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 4        | 4.74          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 9        | 4.73          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 5        | 4.71          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 7        | 4.71          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 1        | 4.71          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 10       | 4.69          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 10       | 4.67          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 3        | 4.66          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 4        | 4.66          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 8        | 4.65          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 8        | 4.65          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 7        | 4.65          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 2        | 4.64          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 2        | 4.64          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 4        | 4.64          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 1        | 4.64          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 1        | 4.61          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 10       | 4.6           |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 4        | 4.6           |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 10       | 4.59          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 9        | 4.57          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 4        | 4.56          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 9        | 4.55          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 1        | 4.55          |
| (1,4)   | 1:18:A:VAL:C | 1:19:A:PHE:N | 1:19:A:PHE:CA | 1:19:A:PHE:C | 5        | 4.55          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 10       | 4.54          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N | 1:32:F:ILE:CA | 1:32:F:ILE:C | 1        | 4.54          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 7        | 4.54          |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 9        | 4.53          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 3        | 4.53          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 5        | 4.52          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 6        | 4.52          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 10       | 4.51          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 9        | 4.5           |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 3        | 4.5           |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 9        | 4.5           |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 10       | 4.48          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 8        | 4.47          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 6        | 4.44          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 7        | 4.44          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 4        | 4.42          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 7        | 4.41          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 3        | 4.39          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 8        | 4.38          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 2        | 4.38          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 4        | 4.38          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 4        | 4.38          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 2        | 4.37          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 6        | 4.35          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 4        | 4.35          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 2        | 4.34          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N | 1:32:G:ILE:CA | 1:32:G:ILE:C | 4        | 4.33          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 2        | 4.33          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 1        | 4.32          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 8        | 4.31          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 9        | 4.31          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 9        | 4.3           |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 3        | 4.29          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N | 1:32:F:ILE:CA | 1:32:F:ILE:C | 10       | 4.28          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 5        | 4.28          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 5        | 4.27          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 2        | 4.27          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 8        | 4.25          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 7        | 4.23          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 9        | 4.22          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 1        | 4.22          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 9        | 4.21          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 5        | 4.21          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 3        | 4.2           |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 2        | 4.2           |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 1        | 4.19          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 1        | 4.18          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 9        | 4.18          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 1        | 4.18          |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 9        | 4.17          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 4        | 4.16          |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 6        | 4.16          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 2        | 4.15          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 9        | 4.15          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 3        | 4.14          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N | 1:32:F:ILE:CA | 1:32:F:ILE:C | 5        | 4.13          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 7        | 4.12          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 6        | 4.12          |
| (1,101) | 1:19:G:PHE:C | 1:20:G:PHE:N | 1:20:G:PHE:CA | 1:20:G:PHE:C | 2        | 4.09          |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 8        | 4.08          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N | 1:32:C:ILE:CA | 1:32:C:ILE:C | 9        | 4.07          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 5        | 4.07          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 3        | 4.06          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 3        | 4.05          |
| (1,5)   | 1:19:A:PHE:C | 1:20:A:PHE:N | 1:20:A:PHE:CA | 1:20:A:PHE:C | 10       | 4.05          |
| (1,117) | 1:19:H:PHE:C | 1:20:H:PHE:N | 1:20:H:PHE:CA | 1:20:H:PHE:C | 5        | 4.04          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 7        | 4.04          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 9        | 4.04          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 7        | 4.03          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 5        | 4.03          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 9        | 4.02          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 5        | 4.01          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N | 1:32:C:ILE:CA | 1:32:C:ILE:C | 2        | 4.0           |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 1        | 3.99          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 4        | 3.98          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 6        | 3.98          |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 2        | 3.96          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 8        | 3.96          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 10       | 3.96          |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 7        | 3.95          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 4        | 3.95          |
| (1,116) | 1:18:H:VAL:C | 1:19:H:PHE:N | 1:19:H:PHE:CA | 1:19:H:PHE:C | 7        | 3.95          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 2        | 3.95          |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 6        | 3.94          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 7        | 3.93          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 6        | 3.92          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 8        | 3.91          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 7        | 3.9           |
| (1,69)  | 1:19:E:PHE:C | 1:20:E:PHE:N | 1:20:E:PHE:CA | 1:20:E:PHE:C | 2        | 3.89          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 9        | 3.89          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 10       | 3.88          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 3        | 3.88          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 3        | 3.88          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 9        | 3.87          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 1        | 3.87          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 8        | 3.87          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 10       | 3.86          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N | 1:32:D:ILE:CA | 1:32:D:ILE:C | 10       | 3.85          |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 2        | 3.85          |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 7        | 3.85          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 3        | 3.85          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 8        | 3.83          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 2        | 3.83          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 8        | 3.83          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 10       | 3.81          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 9        | 3.8           |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 2        | 3.8           |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 3        | 3.79          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 9        | 3.79          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 4        | 3.78          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 9        | 3.78          |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 3        | 3.75          |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 4        | 3.75          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 4        | 3.75          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 7        | 3.75          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 4        | 3.74          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 2        | 3.71          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 6        | 3.7           |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 2        | 3.69          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 5        | 3.69          |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 3        | 3.69          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 10       | 3.67          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 8        | 3.66          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 8        | 3.64          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 2        | 3.63          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 4        | 3.62          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 10       | 3.62          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 8        | 3.6           |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 1        | 3.6           |
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 5        | 3.59          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 2        | 3.59          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 5        | 3.58          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 8        | 3.57          |
| (1,53)  | 1:19:D:PHE:C | 1:20:D:PHE:N | 1:20:D:PHE:CA | 1:20:D:PHE:C | 1        | 3.56          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 9        | 3.56          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 8        | 3.56          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 7        | 3.55          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 1        | 3.53          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 1        | 3.53          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 10       | 3.53          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 5        | 3.52          |
| (1,37)  | 1:19:C:PHE:C | 1:20:C:PHE:N | 1:20:C:PHE:CA | 1:20:C:PHE:C | 9        | 3.52          |
| (1,109) | 1:33:G:GLY:C | 1:34:G:LEU:N | 1:34:G:LEU:CA | 1:34:G:LEU:C | 1        | 3.51          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 4        | 3.5           |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 8        | 3.5           |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 7        | 3.49          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 6        | 3.48          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 1        | 3.48          |
| (1,12)  | 1:32:A:ILE:C | 1:33:A:GLY:N | 1:33:A:GLY:CA | 1:33:A:GLY:C | 6        | 3.47          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 7        | 3.47          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 6        | 3.46          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 10       | 3.46          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 7        | 3.46          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 5        | 3.45          |
| (1,124) | 1:32:H:ILE:C | 1:33:H:GLY:N | 1:33:H:GLY:CA | 1:33:H:GLY:C | 9        | 3.44          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 10       | 3.44          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 3        | 3.43          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,123) | 1:31:H:ILE:C | 1:32:H:ILE:N | 1:32:H:ILE:CA | 1:32:H:ILE:C | 10       | 3.42          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 5        | 3.42          |
| (1,85)  | 1:19:F:PHE:C | 1:20:F:PHE:N | 1:20:F:PHE:CA | 1:20:F:PHE:C | 1        | 3.42          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 6        | 3.4           |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 10       | 3.39          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 1        | 3.39          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 4        | 3.39          |
| (1,76)  | 1:32:E:ILE:C | 1:33:E:GLY:N | 1:33:E:GLY:CA | 1:33:E:GLY:C | 3        | 3.38          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 5        | 3.37          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 6        | 3.34          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 5        | 3.33          |
| (1,108) | 1:32:G:ILE:C | 1:33:G:GLY:N | 1:33:G:GLY:CA | 1:33:G:GLY:C | 10       | 3.33          |
| (1,92)  | 1:32:F:ILE:C | 1:33:F:GLY:N | 1:33:F:GLY:CA | 1:33:F:GLY:C | 5        | 3.33          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 10       | 3.32          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 3        | 3.31          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 8        | 3.3           |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 2        | 3.29          |
| (1,21)  | 1:19:B:PHE:C | 1:20:B:PHE:N | 1:20:B:PHE:CA | 1:20:B:PHE:C | 5        | 3.29          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 6        | 3.28          |
| (1,28)  | 1:32:B:ILE:C | 1:33:B:GLY:N | 1:33:B:GLY:CA | 1:33:B:GLY:C | 3        | 3.27          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 8        | 3.27          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 7        | 3.25          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 6        | 3.23          |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 7        | 3.22          |
| (1,60)  | 1:32:D:ILE:C | 1:33:D:GLY:N | 1:33:D:GLY:CA | 1:33:D:GLY:C | 1        | 3.2           |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 8        | 3.2           |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 3        | 3.2           |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 4        | 3.18          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 7        | 3.17          |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 2        | 3.16          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 3        | 3.15          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 7        | 3.14          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 2        | 3.13          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 5        | 3.12          |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 4        | 3.12          |
| (1,122) | 1:30:H:ALA:C | 1:31:H:ILE:N | 1:31:H:ILE:CA | 1:31:H:ILE:C | 10       | 3.1           |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 10       | 3.1           |
| (1,109) | 1:33:G:GLY:C | 1:34:G:LEU:N | 1:34:G:LEU:CA | 1:34:G:LEU:C | 10       | 3.09          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 9        | 3.04          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 9        | 3.02          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 6        | 3.0           |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 1        | 3.0           |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 3        | 2.99          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 2        | 2.99          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 10       | 2.99          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 6        | 2.97          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 9        | 2.97          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 5        | 2.96          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 4        | 2.94          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 10       | 2.93          |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 5        | 2.93          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N | 1:34:E:LEU:CA | 1:34:E:LEU:C | 9        | 2.89          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 3        | 2.87          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N | 1:34:H:LEU:CA | 1:34:H:LEU:C | 8        | 2.86          |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 6        | 2.86          |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 10       | 2.86          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 5        | 2.85          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 3        | 2.83          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 6        | 2.82          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 6        | 2.82          |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N | 1:34:E:LEU:CA | 1:34:E:LEU:C | 2        | 2.81          |
| (1,10)  | 1:30:A:ALA:C | 1:31:A:ILE:N | 1:31:A:ILE:CA | 1:31:A:ILE:C | 9        | 2.81          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 1        | 2.78          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 4        | 2.78          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 6        | 2.77          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 7        | 2.77          |
| (1,44)  | 1:32:C:ILE:C | 1:33:C:GLY:N | 1:33:C:GLY:CA | 1:33:C:GLY:C | 6        | 2.76          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 1        | 2.75          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 8        | 2.74          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N | 1:18:H:VAL:CA | 1:18:H:VAL:C | 1        | 2.73          |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N | 1:34:E:LEU:CA | 1:34:E:LEU:C | 7        | 2.72          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 4        | 2.72          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 3        | 2.72          |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N | 1:34:A:LEU:CA | 1:34:A:LEU:C | 1        | 2.71          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 8        | 2.7           |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 9        | 2.69          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 7        | 2.68          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N | 1:18:H:VAL:CA | 1:18:H:VAL:C | 4        | 2.66          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 9        | 2.66          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 1        | 2.65          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 6        | 2.62          |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N | 1:34:E:LEU:CA | 1:34:E:LEU:C | 10       | 2.59          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 8        | 2.58          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 8        | 2.54          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 5        | 2.54          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 6        | 2.52          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 9        | 2.52          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 9        | 2.49          |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 6        | 2.49          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 2        | 2.48          |
| (1,84)  | 1:18:F:VAL:C | 1:19:F:PHE:N | 1:19:F:PHE:CA | 1:19:F:PHE:C | 1        | 2.46          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 8        | 2.45          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 2        | 2.45          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 5        | 2.44          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 5        | 2.44          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 3        | 2.43          |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N | 1:34:E:LEU:CA | 1:34:E:LEU:C | 4        | 2.42          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 3        | 2.41          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N | 1:18:H:VAL:CA | 1:18:H:VAL:C | 10       | 2.4           |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 1        | 2.4           |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 5        | 2.39          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 4        | 2.39          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N | 1:34:A:LEU:CA | 1:34:A:LEU:C | 10       | 2.39          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N | 1:34:H:LEU:CA | 1:34:H:LEU:C | 4        | 2.38          |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 8        | 2.38          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 3        | 2.38          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 5        | 2.38          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N | 1:32:G:ILE:CA | 1:32:G:ILE:C | 5        | 2.36          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 9        | 2.36          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 7        | 2.36          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N | 1:34:H:LEU:CA | 1:34:H:LEU:C | 6        | 2.34          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 7        | 2.31          |
| (1,74)  | 1:30:E:ALA:C | 1:31:E:ILE:N | 1:31:E:ILE:CA | 1:31:E:ILE:C | 9        | 2.3           |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 2        | 2.3           |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 4        | 2.27          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N | 1:32:G:ILE:CA | 1:32:G:ILE:C | 1        | 2.26          |
| (1,90)  | 1:30:F:ALA:C | 1:31:F:ILE:N | 1:31:F:ILE:CA | 1:31:F:ILE:C | 4        | 2.25          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 1        | 2.24          |
| (1,30)  | 1:34:B:LEU:C | 1:35:B:MET:N | 1:35:B:MET:CA | 1:35:B:MET:C | 5        | 2.24          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 3        | 2.23          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 3        | 2.22          |
| (1,110) | 1:34:G:LEU:C | 1:35:G:MET:N | 1:35:G:MET:CA | 1:35:G:MET:C | 6        | 2.21          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 7        | 2.21          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 4        | 2.21          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 4        | 2.21          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N | 1:32:C:ILE:CA | 1:32:C:ILE:C | 4        | 2.2           |
| (1,94)  | 1:34:F:LEU:C | 1:35:F:MET:N | 1:35:F:MET:CA | 1:35:F:MET:C | 7        | 2.19          |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 2        | 2.19          |
| (1,36)  | 1:18:C:VAL:C | 1:19:C:PHE:N | 1:19:C:PHE:CA | 1:19:C:PHE:C | 2        | 2.19          |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N | 1:18:G:VAL:CA | 1:18:G:VAL:C | 10       | 2.18          |
| (1,35)  | 1:17:C:LEU:C | 1:18:C:VAL:N | 1:18:C:VAL:CA | 1:18:C:VAL:C | 10       | 2.18          |
| (1,11)  | 1:31:A:ILE:C | 1:32:A:ILE:N | 1:32:A:ILE:CA | 1:32:A:ILE:C | 6        | 2.18          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N | 1:34:H:LEU:CA | 1:34:H:LEU:C | 3        | 2.15          |
| (1,110) | 1:34:G:LEU:C | 1:35:G:MET:N | 1:35:G:MET:CA | 1:35:G:MET:C | 9        | 2.15          |
| (1,58)  | 1:30:D:ALA:C | 1:31:D:ILE:N | 1:31:D:ILE:CA | 1:31:D:ILE:C | 2        | 2.15          |
| (1,26)  | 1:30:B:ALA:C | 1:31:B:ILE:N | 1:31:B:ILE:CA | 1:31:B:ILE:C | 8        | 2.15          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N | 1:18:H:VAL:CA | 1:18:H:VAL:C | 6        | 2.14          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 4        | 2.14          |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 3        | 2.12          |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N | 1:32:E:ILE:CA | 1:32:E:ILE:C | 10       | 2.12          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 4        | 2.12          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N | 1:34:H:LEU:CA | 1:34:H:LEU:C | 7        | 2.11          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 10       | 2.09          |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N | 1:18:E:VAL:CA | 1:18:E:VAL:C | 6        | 2.08          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 9        | 2.08          |
| (1,42)  | 1:30:C:ALA:C | 1:31:C:ILE:N | 1:31:C:ILE:CA | 1:31:C:ILE:C | 3        | 2.07          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 8        | 2.06          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N | 1:32:G:ILE:CA | 1:32:G:ILE:C | 10       | 2.05          |
| (1,110) | 1:34:G:LEU:C | 1:35:G:MET:N | 1:35:G:MET:CA | 1:35:G:MET:C | 5        | 2.04          |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N | 1:18:G:VAL:CA | 1:18:G:VAL:C | 5        | 2.04          |
| (1,106) | 1:30:G:ALA:C | 1:31:G:ILE:N | 1:31:G:ILE:CA | 1:31:G:ILE:C | 2        | 2.03          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 2        | 2.03          |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N | 1:34:E:LEU:CA | 1:34:E:LEU:C | 1        | 2.02          |

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| Key     | Atom-1       | Atom-2       | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|--------------|---------------|--------------|----------|---------------|
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N | 1:32:D:ILE:CA | 1:32:D:ILE:C | 5        | 2.02          |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N | 1:34:A:LEU:CA | 1:34:A:LEU:C | 6        | 2.02          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 9        | 1.99          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N | 1:18:H:VAL:CA | 1:18:H:VAL:C | 7        | 1.98          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 9        | 1.98          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N | 1:32:C:ILE:CA | 1:32:C:ILE:C | 7        | 1.98          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 3        | 1.98          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N | 1:34:H:LEU:CA | 1:34:H:LEU:C | 9        | 1.97          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N | 1:32:F:ILE:CA | 1:32:F:ILE:C | 4        | 1.96          |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 7        | 1.96          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 8        | 1.96          |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N | 1:34:A:LEU:CA | 1:34:A:LEU:C | 5        | 1.96          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 6        | 1.95          |
| (1,35)  | 1:17:C:LEU:C | 1:18:C:VAL:N | 1:18:C:VAL:CA | 1:18:C:VAL:C | 6        | 1.95          |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N | 1:34:B:LEU:CA | 1:34:B:LEU:C | 1        | 1.95          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N | 1:32:D:ILE:CA | 1:32:D:ILE:C | 4        | 1.94          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 9        | 1.94          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N | 1:32:D:ILE:CA | 1:32:D:ILE:C | 8        | 1.93          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N | 1:32:C:ILE:CA | 1:32:C:ILE:C | 6        | 1.93          |
| (1,35)  | 1:17:C:LEU:C | 1:18:C:VAL:N | 1:18:C:VAL:CA | 1:18:C:VAL:C | 5        | 1.92          |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 4        | 1.9           |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N | 1:18:E:VAL:CA | 1:18:E:VAL:C | 9        | 1.9           |
| (1,109) | 1:33:G:GLY:C | 1:34:G:LEU:N | 1:34:G:LEU:CA | 1:34:G:LEU:C | 2        | 1.88          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 10       | 1.87          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 4        | 1.86          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 2        | 1.86          |
| (1,110) | 1:34:G:LEU:C | 1:35:G:MET:N | 1:35:G:MET:CA | 1:35:G:MET:C | 7        | 1.85          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 2        | 1.85          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N | 1:32:D:ILE:CA | 1:32:D:ILE:C | 1        | 1.85          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 7        | 1.85          |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N | 1:18:E:VAL:CA | 1:18:E:VAL:C | 1        | 1.84          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N | 1:32:D:ILE:CA | 1:32:D:ILE:C | 7        | 1.84          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 2        | 1.84          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N | 1:18:H:VAL:CA | 1:18:H:VAL:C | 3        | 1.82          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 3        | 1.81          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N | 1:34:F:LEU:CA | 1:34:F:LEU:C | 1        | 1.8           |
| (1,94)  | 1:34:F:LEU:C | 1:35:F:MET:N | 1:35:F:MET:CA | 1:35:F:MET:C | 6        | 1.78          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 10       | 1.78          |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N | 1:18:G:VAL:CA | 1:18:G:VAL:C | 4        | 1.77          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N | 1:32:B:ILE:CA | 1:32:B:ILE:C | 6        | 1.77          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N | 1:34:C:LEU:CA | 1:34:C:LEU:C | 5        | 1.76          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N | 1:32:F:ILE:CA | 1:32:F:ILE:C | 9        | 1.74          |
| (1,83)  | 1:17:F:LEU:C | 1:18:F:VAL:N | 1:18:F:VAL:CA | 1:18:F:VAL:C | 9        | 1.74          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N | 1:18:B:VAL:CA | 1:18:B:VAL:C | 1        | 1.74          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 5        | 1.74          |
| (1,78)  | 1:34:E:LEU:C | 1:35:E:MET:N | 1:35:E:MET:CA | 1:35:E:MET:C | 6        | 1.73          |
| (1,61)  | 1:33:D:GLY:C | 1:34:D:LEU:N | 1:34:D:LEU:CA | 1:34:D:LEU:C | 7        | 1.73          |
| (1,46)  | 1:34:C:LEU:C | 1:35:C:MET:N | 1:35:C:MET:CA | 1:35:C:MET:C | 10       | 1.73          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N | 1:18:A:VAL:CA | 1:18:A:VAL:C | 10       | 1.73          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N | 1:32:F:ILE:CA | 1:32:F:ILE:C | 2        | 1.72          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N | 1:18:D:VAL:CA | 1:18:D:VAL:C | 8        | 1.72          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N  | 1:34:E:LEU:CA | 1:34:E:LEU:C | 5        | 1.71          |
| (1,46)  | 1:34:C:LEU:C | 1:35:C:MET:N  | 1:35:C:MET:CA | 1:35:C:MET:C | 6        | 1.71          |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N  | 1:18:E:VAL:CA | 1:18:E:VAL:C | 10       | 1.7           |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N  | 1:32:C:ILE:CA | 1:32:C:ILE:C | 5        | 1.7           |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N  | 1:18:G:VAL:CA | 1:18:G:VAL:C | 7        | 1.69          |
| (1,62)  | 1:34:D:LEU:C | 1:35:D:MET:N  | 1:35:D:MET:CA | 1:35:D:MET:C | 10       | 1.69          |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N  | 1:18:G:VAL:CA | 1:18:G:VAL:C | 2        | 1.66          |
| (1,35)  | 1:17:C:LEU:C | 1:18:C:VAL:N  | 1:18:C:VAL:CA | 1:18:C:VAL:C | 8        | 1.66          |
| (1,29)  | 1:33:B:GLY:C | 1:34:B:LEU:N  | 1:34:B:LEU:CA | 1:34:B:LEU:C | 6        | 1.66          |
| (1,94)  | 1:34:F:LEU:C | 1:35:F:MET:N  | 1:35:F:MET:CA | 1:35:F:MET:C | 8        | 1.64          |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N  | 1:18:E:VAL:CA | 1:18:E:VAL:C | 5        | 1.64          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N  | 1:18:D:VAL:CA | 1:18:D:VAL:C | 2        | 1.64          |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N  | 1:18:E:VAL:CA | 1:18:E:VAL:C | 3        | 1.63          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N  | 1:32:C:ILE:CA | 1:32:C:ILE:C | 1        | 1.63          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N  | 1:32:C:ILE:CA | 1:32:C:ILE:C | 3        | 1.63          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N  | 1:32:F:ILE:CA | 1:32:F:ILE:C | 8        | 1.62          |
| (1,137) | 1:30:A:ALA:N | 1:30:A:ALA:CA | 1:30:A:ALA:C  | 1:31:A:ILE:N | 8        | 1.61          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N  | 1:32:G:ILE:CA | 1:32:G:ILE:C | 7        | 1.6           |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N  | 1:18:G:VAL:CA | 1:18:G:VAL:C | 1        | 1.6           |
| (1,75)  | 1:31:E:ILE:C | 1:32:E:ILE:N  | 1:32:E:ILE:CA | 1:32:E:ILE:C | 1        | 1.6           |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N  | 1:32:G:ILE:CA | 1:32:G:ILE:C | 9        | 1.59          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N  | 1:32:D:ILE:CA | 1:32:D:ILE:C | 3        | 1.58          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N  | 1:32:G:ILE:CA | 1:32:G:ILE:C | 2        | 1.55          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N  | 1:34:F:LEU:CA | 1:34:F:LEU:C | 3        | 1.55          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N  | 1:18:H:VAL:CA | 1:18:H:VAL:C | 9        | 1.54          |
| (1,67)  | 1:17:E:LEU:C | 1:18:E:VAL:N  | 1:18:E:VAL:CA | 1:18:E:VAL:C | 7        | 1.54          |
| (1,109) | 1:33:G:GLY:C | 1:34:G:LEU:N  | 1:34:G:LEU:CA | 1:34:G:LEU:C | 8        | 1.53          |
| (1,94)  | 1:34:F:LEU:C | 1:35:F:MET:N  | 1:35:F:MET:CA | 1:35:F:MET:C | 5        | 1.53          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N  | 1:18:A:VAL:CA | 1:18:A:VAL:C | 6        | 1.53          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N  | 1:18:H:VAL:CA | 1:18:H:VAL:C | 5        | 1.51          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N  | 1:32:C:ILE:CA | 1:32:C:ILE:C | 8        | 1.49          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N  | 1:18:H:VAL:CA | 1:18:H:VAL:C | 8        | 1.47          |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N  | 1:34:E:LEU:CA | 1:34:E:LEU:C | 8        | 1.45          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N  | 1:32:G:ILE:CA | 1:32:G:ILE:C | 6        | 1.44          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N  | 1:18:A:VAL:CA | 1:18:A:VAL:C | 1        | 1.44          |
| (1,115) | 1:17:H:LEU:C | 1:18:H:VAL:N  | 1:18:H:VAL:CA | 1:18:H:VAL:C | 2        | 1.43          |
| (1,30)  | 1:34:B:LEU:C | 1:35:B:MET:N  | 1:35:B:MET:CA | 1:35:B:MET:C | 1        | 1.43          |
| (1,78)  | 1:34:E:LEU:C | 1:35:E:MET:N  | 1:35:E:MET:CA | 1:35:E:MET:C | 7        | 1.42          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N  | 1:32:D:ILE:CA | 1:32:D:ILE:C | 9        | 1.41          |
| (1,201) | 1:30:E:ALA:N | 1:30:E:ALA:CA | 1:30:E:ALA:C  | 1:31:E:ILE:N | 5        | 1.4           |
| (1,118) | 1:20:H:PHE:C | 1:21:H:ALA:N  | 1:21:H:ALA:CA | 1:21:H:ALA:C | 8        | 1.4           |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N  | 1:34:H:LEU:CA | 1:34:H:LEU:C | 1        | 1.39          |
| (1,3)   | 1:17:A:LEU:C | 1:18:A:VAL:N  | 1:18:A:VAL:CA | 1:18:A:VAL:C | 8        | 1.38          |
| (1,46)  | 1:34:C:LEU:C | 1:35:C:MET:N  | 1:35:C:MET:CA | 1:35:C:MET:C | 2        | 1.37          |
| (1,46)  | 1:34:C:LEU:C | 1:35:C:MET:N  | 1:35:C:MET:CA | 1:35:C:MET:C | 4        | 1.37          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N  | 1:34:H:LEU:CA | 1:34:H:LEU:C | 5        | 1.34          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N  | 1:18:B:VAL:CA | 1:18:B:VAL:C | 10       | 1.33          |
| (1,109) | 1:33:G:GLY:C | 1:34:G:LEU:N  | 1:34:G:LEU:CA | 1:34:G:LEU:C | 3        | 1.32          |
| (1,109) | 1:33:G:GLY:C | 1:34:G:LEU:N  | 1:34:G:LEU:CA | 1:34:G:LEU:C | 5        | 1.32          |
| (1,19)  | 1:17:B:LEU:C | 1:18:B:VAL:N  | 1:18:B:VAL:CA | 1:18:B:VAL:C | 5        | 1.32          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N  | 1:32:F:ILE:CA | 1:32:F:ILE:C | 6        | 1.31          |

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| Key     | Atom-1       | Atom-2        | Atom-3        | Atom-4       | Model ID | Violation (°) |
|---------|--------------|---------------|---------------|--------------|----------|---------------|
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N  | 1:32:G:ILE:CA | 1:32:G:ILE:C | 3        | 1.3           |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N  | 1:34:A:LEU:CA | 1:34:A:LEU:C | 3        | 1.3           |
| (1,30)  | 1:34:B:LEU:C | 1:35:B:MET:N  | 1:35:B:MET:CA | 1:35:B:MET:C | 10       | 1.27          |
| (1,94)  | 1:34:F:LEU:C | 1:35:F:MET:N  | 1:35:F:MET:CA | 1:35:F:MET:C | 3        | 1.26          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N  | 1:32:B:ILE:CA | 1:32:B:ILE:C | 4        | 1.26          |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N  | 1:18:G:VAL:CA | 1:18:G:VAL:C | 3        | 1.25          |
| (1,45)  | 1:33:C:GLY:C | 1:34:C:LEU:N  | 1:34:C:LEU:CA | 1:34:C:LEU:C | 6        | 1.24          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N  | 1:34:H:LEU:CA | 1:34:H:LEU:C | 2        | 1.23          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N  | 1:32:F:ILE:CA | 1:32:F:ILE:C | 3        | 1.23          |
| (1,43)  | 1:31:C:ILE:C | 1:32:C:ILE:N  | 1:32:C:ILE:CA | 1:32:C:ILE:C | 10       | 1.23          |
| (1,174) | 1:35:C:MET:N | 1:35:C:MET:CA | 1:35:C:MET:C  | 1:36:C:VAL:N | 2        | 1.22          |
| (1,93)  | 1:33:F:GLY:C | 1:34:F:LEU:N  | 1:34:F:LEU:CA | 1:34:F:LEU:C | 8        | 1.19          |
| (1,30)  | 1:34:B:LEU:C | 1:35:B:MET:N  | 1:35:B:MET:CA | 1:35:B:MET:C | 2        | 1.19          |
| (1,77)  | 1:33:E:GLY:C | 1:34:E:LEU:N  | 1:34:E:LEU:CA | 1:34:E:LEU:C | 3        | 1.17          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N  | 1:32:D:ILE:CA | 1:32:D:ILE:C | 2        | 1.14          |
| (1,125) | 1:33:H:GLY:C | 1:34:H:LEU:N  | 1:34:H:LEU:CA | 1:34:H:LEU:C | 10       | 1.13          |
| (1,99)  | 1:17:G:LEU:C | 1:18:G:VAL:N  | 1:18:G:VAL:CA | 1:18:G:VAL:C | 9        | 1.12          |
| (1,62)  | 1:34:D:LEU:C | 1:35:D:MET:N  | 1:35:D:MET:CA | 1:35:D:MET:C | 6        | 1.12          |
| (1,27)  | 1:31:B:ILE:C | 1:32:B:ILE:N  | 1:32:B:ILE:CA | 1:32:B:ILE:C | 7        | 1.12          |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N  | 1:34:A:LEU:CA | 1:34:A:LEU:C | 8        | 1.12          |
| (1,107) | 1:31:G:ILE:C | 1:32:G:ILE:N  | 1:32:G:ILE:CA | 1:32:G:ILE:C | 8        | 1.11          |
| (1,14)  | 1:34:A:LEU:C | 1:35:A:MET:N  | 1:35:A:MET:CA | 1:35:A:MET:C | 2        | 1.11          |
| (1,46)  | 1:34:C:LEU:C | 1:35:C:MET:N  | 1:35:C:MET:CA | 1:35:C:MET:C | 8        | 1.08          |
| (1,35)  | 1:17:C:LEU:C | 1:18:C:VAL:N  | 1:18:C:VAL:CA | 1:18:C:VAL:C | 3        | 1.08          |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N  | 1:34:A:LEU:CA | 1:34:A:LEU:C | 7        | 1.08          |
| (1,91)  | 1:31:F:ILE:C | 1:32:F:ILE:N  | 1:32:F:ILE:CA | 1:32:F:ILE:C | 7        | 1.06          |
| (1,94)  | 1:34:F:LEU:C | 1:35:F:MET:N  | 1:35:F:MET:CA | 1:35:F:MET:C | 9        | 1.05          |
| (1,110) | 1:34:G:LEU:C | 1:35:G:MET:N  | 1:35:G:MET:CA | 1:35:G:MET:C | 8        | 1.04          |
| (1,51)  | 1:17:D:LEU:C | 1:18:D:VAL:N  | 1:18:D:VAL:CA | 1:18:D:VAL:C | 5        | 1.02          |
| (1,13)  | 1:33:A:GLY:C | 1:34:A:LEU:N  | 1:34:A:LEU:CA | 1:34:A:LEU:C | 2        | 1.02          |
| (1,59)  | 1:31:D:ILE:C | 1:32:D:ILE:N  | 1:32:D:ILE:CA | 1:32:D:ILE:C | 6        | 1.01          |