



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 06:58 AM UTC

PDB ID : 2N3U / pdb\_00002n3u  
BMRB ID : 25657  
Title : Solution structure of the Rpn1 T1 site engaging two monoubiquitin molecules  
Authors : Chen, X.; Walters, K.J.  
Deposited on : 2015-06-10

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 : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

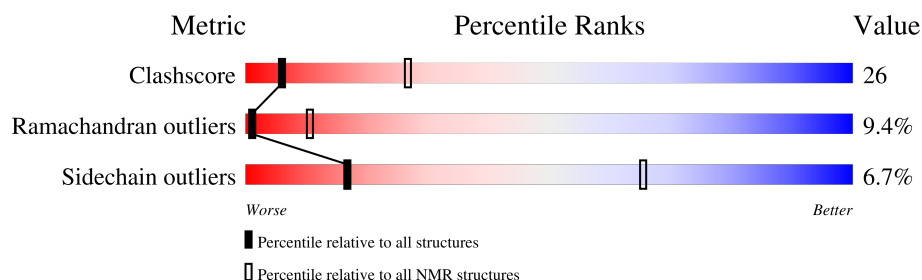
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 28%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 229148                      | 14424                     |
| Ramachandran outliers | 224038                      | 12848                     |
| Sidechain outliers    | 223484                      | 12823                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 131    |                  |
| 2   | B     | 76     |                  |
| 2   | C     | 76     |                  |

## 2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                       |                   |              |
|--------------------------------------|---------------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)                 | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:486-A:607, B:1-B:76, C:1-C:72 (270) | 1.24              | 2            |

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 and 2 single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 4383 atoms, of which 2225 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome regulatory subunit RPN1.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 1   | A     | 131      | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1921  | 606 | 967 | 150 | 192 | 6 |       |

- Molecule 2 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |     |     |     |   | Trace |
|-----|-------|----------|-------|-----|-----|-----|-----|---|-------|
| 2   | B     | 76       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1231  | 378 | 629 | 105 | 118 | 1 |       |
| 2   | C     | 76       | Total | C   | H   | N   | O   | S | 0     |
|     |       |          | 1231  | 378 | 629 | 105 | 118 | 1 |       |

## 4 Residue-property plots

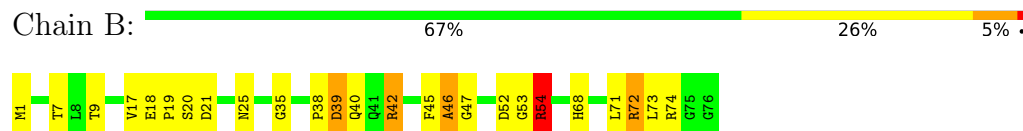
### 4.1 Average score per residue in the NMR ensemble

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

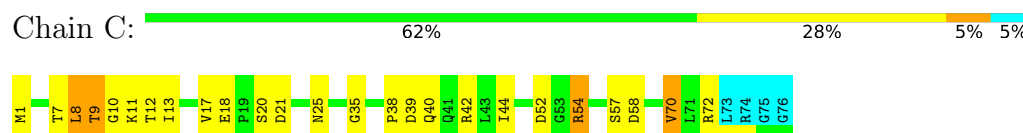
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40



- Molecule 2: Ubiquitin-60S ribosomal protein L40



### 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: 26S proteasome regulatory subunit RPN1





- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 57% 37% 5%



- Molecule 2: Ubiquitin-60S ribosomal protein L40

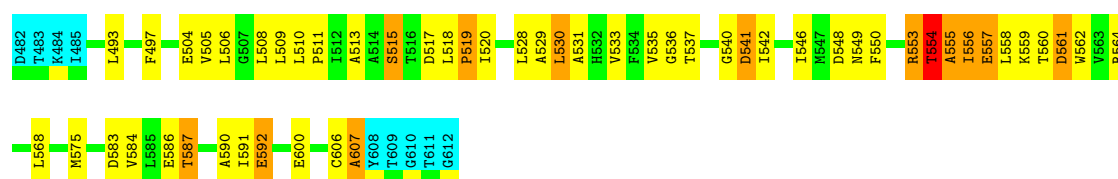
Chain C: 62% 26% 5% 5%



#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 53% 31% 9% 7%



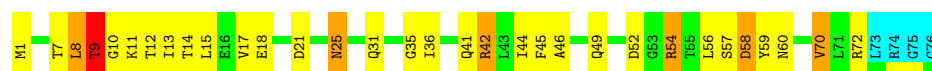
- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 57% 32% 9%



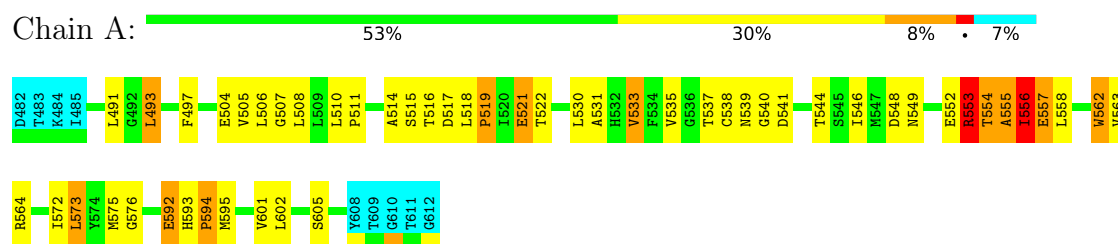
- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain C: 53% 33% 8% 5%

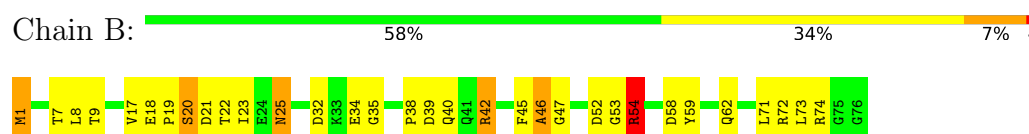


#### 4.2.3 Score per residue for model 3

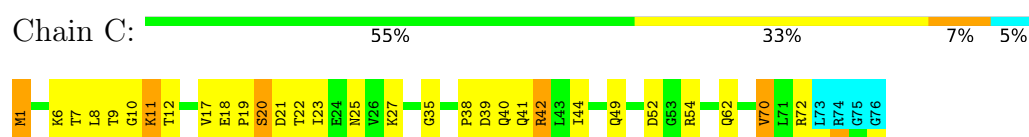
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

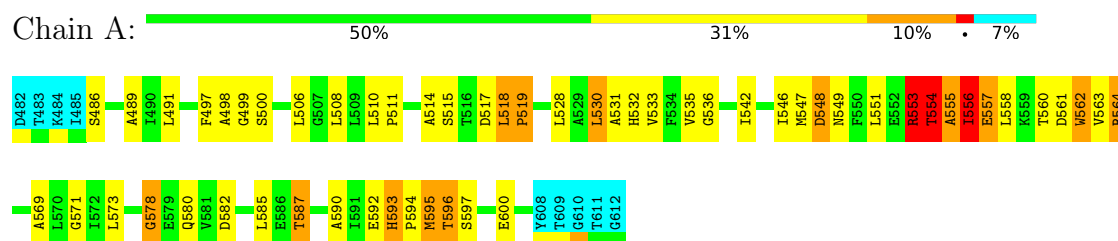


- Molecule 2: Ubiquitin-60S ribosomal protein L40

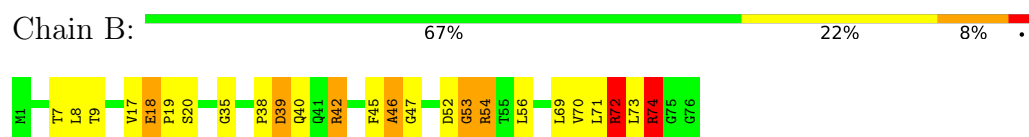


#### 4.2.4 Score per residue for model 4

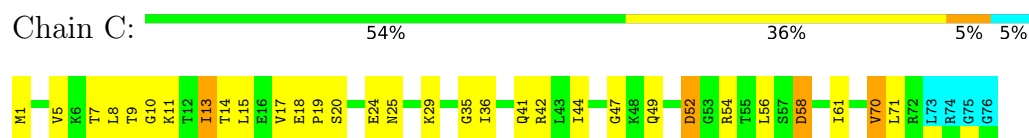
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

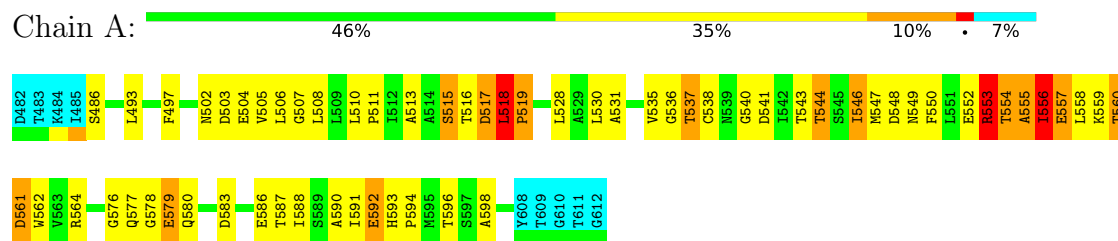


- Molecule 2: Ubiquitin-60S ribosomal protein L40

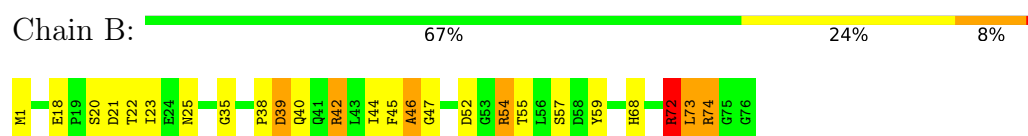


### 4.2.5 Score per residue for model 5

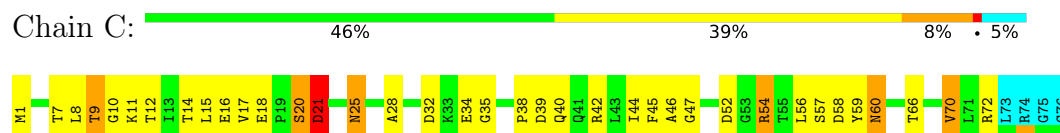
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

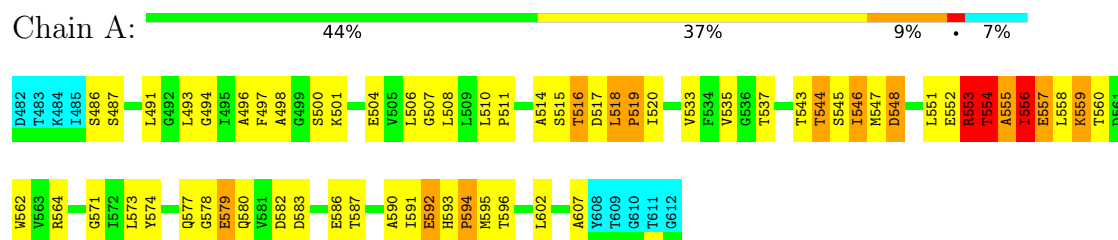


- Molecule 2: Ubiquitin-60S ribosomal protein L40

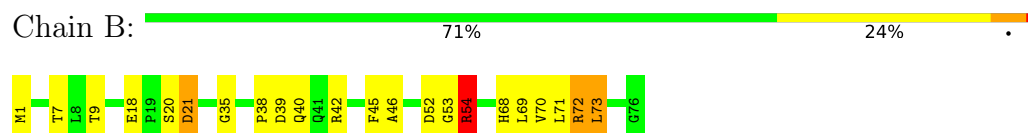


### 4.2.6 Score per residue for model 6

- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

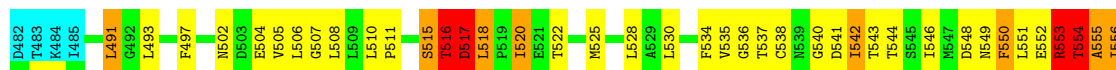




#### 4.2.7 Score per residue for model 7

- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 47% 37% 7% 7%



- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 62% 33% 5%



- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain C: 63% 28% 9%



#### 4.2.8 Score per residue for model 8

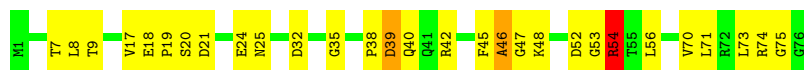
- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 44% 41% 7% 7%

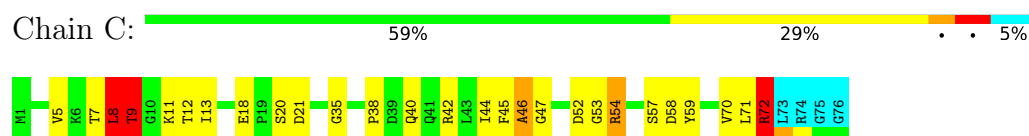


- Molecule 2: Ubiquitin-60S ribosomal protein L40

Chain B: 62% 34% 4%



- Molecule 2: Ubiquitin-60S ribosomal protein L40

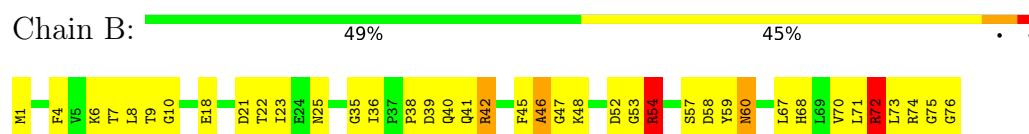


#### 4.2.9 Score per residue for model 9

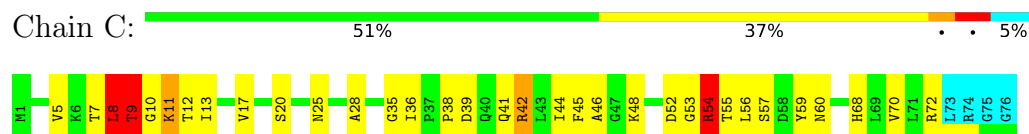
- Molecule 1: 26S proteasome regulatory subunit RPN1



- Molecule 2: Ubiquitin-60S ribosomal protein L40

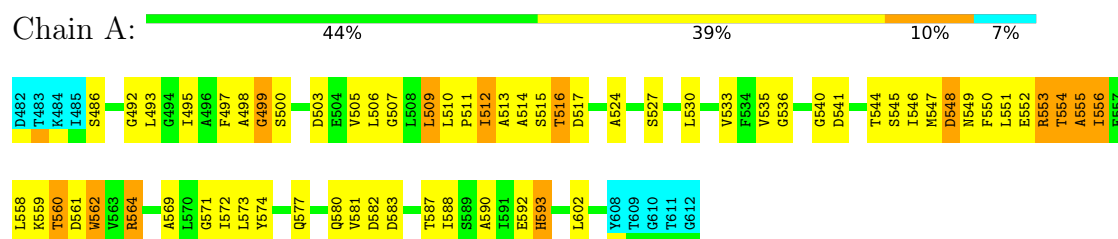


- Molecule 2: Ubiquitin-60S ribosomal protein L40



#### 4.2.10 Score per residue for model 10

- Molecule 1: 26S proteasome regulatory subunit RPN1

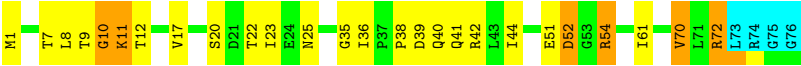


- Molecule 2: Ubiquitin-60S ribosomal protein L40





● Molecule 2: Ubiquitin-60S ribosomal protein L40



## 5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 10 were deposited, based on the following criterion: ?.

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

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

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                       | 1034           |
| Number of shifts mapped to atoms             | 1034           |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 0              |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 28%            |

## 6 Model quality i

### 6.1 Standard geometry i

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

| Mol | Chain | Bond lengths |                      | Bond angles |                       |
|-----|-------|--------------|----------------------|-------------|-----------------------|
|     |       | RMSZ         | #Z>5                 | RMSZ        | #Z>5                  |
| 1   | A     | 0.55±0.03    | 0±0/899 ( 0.0± 0.1%) | 0.96±0.03   | 1±1/1226 ( 0.1± 0.1%) |
| 2   | B     | 0.55±0.01    | 0±0/608 ( 0.0± 0.0%) | 1.01±0.02   | 0±0/816 ( 0.0± 0.0%)  |
| 2   | C     | 0.55±0.00    | 0±0/581 ( 0.0± 0.0%) | 1.03±0.02   | 0±0/784 ( 0.0± 0.0%)  |
| All | All   | 0.55         | 3/20880 ( 0.0%)      | 0.99        | 12/28260 ( 0.0%)      |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | Chirality | Planarity |
|-----|-------|-----------|-----------|
| 1   | A     | 0.0±0.0   | 1.8±0.4   |
| 2   | B     | 0.0±0.0   | 3.3±0.6   |
| 2   | C     | 0.0±0.0   | 2.5±0.7   |
| All | All   | 0         | 76        |

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|-------|-------|-------------|----------|--------|-------|
|     |       |     |      |       |       |             |          | Worst  | Total |
| 1   | A     | 556 | ILE  | C-O   | -9.52 | 1.12        | 1.24     | 1      | 1     |
| 1   | A     | 553 | ARG  | C-N   | -5.15 | 1.26        | 1.33     | 3      | 1     |
| 1   | A     | 554 | THR  | N-CA  | 5.12  | 1.52        | 1.46     | 4      | 1     |

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|--------|-------|-------------|----------|--------|-------|
|     |       |     |      |        |       |             |          | Worst  | Total |
| 1   | A     | 553 | ARG  | CA-C-N | 7.68  | 136.22      | 121.54   | 4      | 1     |
| 1   | A     | 553 | ARG  | C-N-CA | 7.68  | 136.22      | 121.54   | 4      | 1     |
| 2   | B     | 21  | ASP  | N-CA-C | -7.42 | 97.49       | 109.96   | 6      | 1     |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|---------|-------|-------------|----------|--------|-------|
|     |       |     |      |         |       |             |          | Worst  | Total |
| 1   | A     | 557 | GLU  | N-CA-C  | -6.55 | 98.97       | 109.39   | 3      | 1     |
| 1   | A     | 554 | THR  | N-CA-C  | -6.20 | 97.59       | 110.80   | 1      | 3     |
| 2   | C     | 9   | THR  | N-CA-C  | 5.74  | 117.63      | 110.91   | 5      | 1     |
| 1   | A     | 553 | ARG  | N-CA-C  | -5.71 | 98.63       | 110.80   | 9      | 2     |
| 1   | A     | 556 | ILE  | O-C-N   | 5.37  | 129.29      | 122.57   | 1      | 1     |
| 1   | A     | 607 | ALA  | CB-CA-C | -5.23 | 109.56      | 115.79   | 9      | 1     |

There are no chirality outliers.

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

| Mol | Chain | Res | Type | Group     | Models (Total) |
|-----|-------|-----|------|-----------|----------------|
| 1   | A     | 564 | ARG  | Sidechain | 10             |
| 2   | B     | 42  | ARG  | Sidechain | 9              |
| 2   | B     | 54  | ARG  | Sidechain | 9              |
| 2   | C     | 54  | ARG  | Sidechain | 9              |
| 2   | B     | 74  | ARG  | Sidechain | 8              |
| 2   | C     | 42  | ARG  | Sidechain | 8              |
| 1   | A     | 553 | ARG  | Sidechain | 8              |
| 2   | C     | 72  | ARG  | Sidechain | 8              |
| 2   | B     | 72  | ARG  | Sidechain | 7              |

## 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     | 887   | 901      | 901      | 64±9    |
| 2   | B     | 602   | 629      | 629      | 28±6    |
| 2   | C     | 574   | 599      | 599      | 24±4    |
| All | All   | 20630 | 21290    | 21290    | 1108    |

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 26.

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

| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:553:ARG:O    | 1:A:554:THR:C   | 0.91     | 2.13        | 2      | 6     |
| 2:C:7:THR:HG23   | 2:C:11:LYS:O    | 0.89     | 1.68        | 1      | 7     |
| 1:A:554:THR:C    | 1:A:556:ILE:H   | 0.85     | 1.79        | 3      | 4     |
| 2:C:44:ILE:HD12  | 2:C:70:VAL:HG21 | 0.83     | 1.49        | 3      | 10    |
| 2:B:15:LEU:HD22  | 2:B:15:LEU:N    | 0.82     | 1.90        | 10     | 1     |
| 2:C:8:LEU:O      | 2:C:9:THR:HG23  | 0.81     | 1.75        | 9      | 7     |
| 1:A:583:ASP:CG   | 2:B:68:HIS:HE2  | 0.78     | 1.86        | 10     | 3     |
| 2:B:73:LEU:HD22  | 2:B:73:LEU:H    | 0.77     | 1.37        | 7      | 7     |
| 1:A:554:THR:O    | 1:A:555:ALA:C   | 0.76     | 2.27        | 7      | 7     |
| 2:B:73:LEU:HD22  | 2:B:73:LEU:N    | 0.75     | 1.96        | 2      | 7     |
| 1:A:553:ARG:O    | 1:A:555:ALA:N   | 0.75     | 2.20        | 3      | 6     |
| 1:A:554:THR:O    | 1:A:556:ILE:N   | 0.74     | 2.20        | 10     | 10    |
| 1:A:556:ILE:O    | 1:A:558:LEU:N   | 0.74     | 2.20        | 9      | 9     |
| 1:A:555:ALA:O    | 1:A:557:GLU:N   | 0.74     | 2.21        | 3      | 6     |
| 1:A:578:GLY:O    | 1:A:580:GLN:N   | 0.74     | 2.21        | 6      | 3     |
| 1:A:556:ILE:O    | 1:A:557:GLU:C   | 0.72     | 2.32        | 5      | 7     |
| 1:A:554:THR:C    | 1:A:556:ILE:N   | 0.72     | 2.44        | 3      | 8     |
| 2:B:69:LEU:C     | 2:B:69:LEU:HD23 | 0.72     | 2.09        | 2      | 3     |
| 1:A:555:ALA:O    | 1:A:556:ILE:C   | 0.72     | 2.32        | 9      | 4     |
| 1:A:554:THR:O    | 1:A:556:ILE:HB  | 0.69     | 1.86        | 1      | 2     |
| 1:A:555:ALA:C    | 1:A:557:GLU:H   | 0.69     | 1.94        | 3      | 3     |
| 1:A:511:PRO:O    | 1:A:515:SER:N   | 0.69     | 2.25        | 10     | 8     |
| 2:C:11:LYS:HG2   | 2:C:12:THR:N    | 0.68     | 2.02        | 7      | 1     |
| 2:B:71:LEU:HD23  | 2:B:71:LEU:N    | 0.68     | 2.04        | 9      | 1     |
| 1:A:495:ILE:HD12 | 1:A:495:ILE:C   | 0.67     | 2.15        | 10     | 1     |
| 2:C:7:THR:OG1    | 2:C:10:GLY:N    | 0.66     | 2.27        | 1      | 4     |
| 1:A:512:ILE:HD11 | 2:C:9:THR:OG1   | 0.66     | 1.90        | 8      | 1     |
| 2:B:73:LEU:H     | 2:B:73:LEU:CD2  | 0.65     | 2.04        | 9      | 6     |
| 2:C:15:LEU:N     | 2:C:15:LEU:HD22 | 0.64     | 2.07        | 6      | 2     |
| 1:A:578:GLY:C    | 1:A:580:GLN:N   | 0.64     | 2.55        | 5      | 3     |
| 1:A:543:THR:O    | 1:A:544:THR:C   | 0.64     | 2.41        | 6      | 2     |
| 2:B:45:PHE:CG    | 2:B:46:ALA:N    | 0.63     | 2.66        | 5      | 9     |
| 1:A:549:ASN:O    | 1:A:553:ARG:N   | 0.63     | 2.32        | 7      | 8     |
| 1:A:553:ARG:O    | 1:A:556:ILE:N   | 0.63     | 2.31        | 8      | 2     |
| 1:A:562:TRP:CG   | 1:A:563:VAL:N   | 0.63     | 2.67        | 4      | 3     |
| 2:B:18:GLU:H     | 2:B:21:ASP:CG   | 0.63     | 2.02        | 10     | 7     |
| 1:A:543:THR:O    | 1:A:546:ILE:N   | 0.62     | 2.32        | 6      | 2     |
| 1:A:562:TRP:CD1  | 1:A:563:VAL:N   | 0.62     | 2.67        | 9      | 1     |
| 2:C:8:LEU:C      | 2:C:9:THR:HG23  | 0.62     | 2.19        | 5      | 1     |
| 2:B:38:PRO:C     | 2:B:40:GLN:H    | 0.61     | 2.03        | 3      | 7     |
| 2:B:69:LEU:HD23  | 2:B:70:VAL:N    | 0.61     | 2.09        | 6      | 3     |
| 2:B:70:VAL:HG12  | 2:B:71:LEU:H    | 0.61     | 1.53        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:555:ALA:C    | 1:A:557:GLU:N    | 0.61     | 2.56        | 3      | 5     |
| 2:C:11:LYS:CG    | 2:C:12:THR:N     | 0.61     | 2.64        | 8      | 8     |
| 1:A:518:LEU:N    | 1:A:518:LEU:CD2  | 0.60     | 2.64        | 2      | 2     |
| 2:B:15:LEU:N     | 2:B:15:LEU:CD2   | 0.60     | 2.62        | 10     | 1     |
| 1:A:518:LEU:HD12 | 1:A:518:LEU:O    | 0.60     | 1.96        | 4      | 3     |
| 1:A:509:LEU:C    | 1:A:509:LEU:HD23 | 0.60     | 2.21        | 2      | 1     |
| 2:C:45:PHE:CG    | 2:C:46:ALA:N     | 0.60     | 2.70        | 5      | 3     |
| 1:A:556:ILE:O    | 1:A:556:ILE:HG23 | 0.60     | 1.95        | 7      | 4     |
| 2:C:7:THR:OG1    | 2:C:11:LYS:N     | 0.59     | 2.34        | 10     | 7     |
| 1:A:520:ILE:HD11 | 1:A:555:ALA:O    | 0.59     | 1.97        | 2      | 2     |
| 2:B:54:ARG:N     | 2:B:54:ARG:HE    | 0.59     | 1.94        | 2      | 1     |
| 1:A:551:LEU:N    | 1:A:551:LEU:HD12 | 0.59     | 2.12        | 9      | 4     |
| 1:A:556:ILE:O    | 1:A:558:LEU:O    | 0.59     | 2.20        | 6      | 3     |
| 1:A:511:PRO:O    | 1:A:514:ALA:N    | 0.58     | 2.36        | 10     | 2     |
| 2:B:71:LEU:N     | 2:B:71:LEU:CD2   | 0.58     | 2.66        | 9      | 1     |
| 2:C:7:THR:O      | 2:C:8:LEU:C      | 0.58     | 2.46        | 8      | 9     |
| 1:A:575:MET:SD   | 1:A:576:GLY:N    | 0.58     | 2.76        | 3      | 1     |
| 2:B:70:VAL:HG12  | 2:B:71:LEU:N     | 0.58     | 2.13        | 9      | 2     |
| 2:C:36:ILE:O     | 2:C:41:GLN:NE2   | 0.58     | 2.37        | 4      | 4     |
| 1:A:515:SER:O    | 1:A:516:THR:CB   | 0.58     | 2.52        | 9      | 3     |
| 2:B:45:PHE:O     | 2:B:47:GLY:N     | 0.58     | 2.37        | 2      | 7     |
| 2:C:14:THR:C     | 2:C:15:LEU:HD12  | 0.57     | 2.24        | 2      | 2     |
| 2:C:42:ARG:NE    | 2:C:49:GLN:NE2   | 0.57     | 2.52        | 3      | 1     |
| 1:A:514:ALA:C    | 1:A:516:THR:H    | 0.57     | 2.08        | 10     | 1     |
| 1:A:551:LEU:N    | 1:A:551:LEU:CD1  | 0.57     | 2.67        | 9      | 2     |
| 2:C:38:PRO:C     | 2:C:40:GLN:H     | 0.57     | 2.07        | 5      | 6     |
| 1:A:554:THR:O    | 1:A:556:ILE:CB   | 0.57     | 2.52        | 1      | 1     |
| 2:B:73:LEU:N     | 2:B:73:LEU:CD2   | 0.57     | 2.67        | 10     | 6     |
| 2:C:8:LEU:O      | 2:C:9:THR:OG1    | 0.57     | 2.17        | 5      | 2     |
| 1:A:518:LEU:N    | 1:A:518:LEU:HD22 | 0.57     | 2.15        | 2      | 1     |
| 1:A:578:GLY:O    | 1:A:579:GLU:C    | 0.56     | 2.48        | 6      | 2     |
| 1:A:593:HIS:N    | 1:A:593:HIS:ND1  | 0.56     | 2.50        | 10     | 2     |
| 2:B:36:ILE:O     | 2:B:41:GLN:NE2   | 0.56     | 2.38        | 2      | 2     |
| 2:B:45:PHE:CD2   | 2:B:46:ALA:N     | 0.56     | 2.74        | 3      | 4     |
| 2:C:8:LEU:HD13   | 2:C:70:VAL:HG13  | 0.56     | 1.78        | 2      | 1     |
| 1:A:518:LEU:HD23 | 1:A:518:LEU:N    | 0.56     | 2.15        | 7      | 1     |
| 1:A:511:PRO:O    | 1:A:513:ALA:N    | 0.56     | 2.38        | 10     | 2     |
| 1:A:497:PHE:CD1  | 1:A:497:PHE:C    | 0.56     | 2.83        | 9      | 1     |
| 2:B:1:MET:N      | 2:B:17:VAL:O     | 0.56     | 2.38        | 2      | 4     |
| 1:A:510:LEU:HB3  | 1:A:511:PRO:CD   | 0.56     | 2.30        | 10     | 8     |
| 1:A:506:LEU:O    | 1:A:508:LEU:N    | 0.56     | 2.39        | 6      | 6     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:493:LEU:O    | 1:A:497:PHE:CD2  | 0.56     | 2.59        | 6      | 3     |
| 2:B:71:LEU:HD12  | 2:B:71:LEU:N     | 0.55     | 2.16        | 3      | 2     |
| 2:C:15:LEU:N     | 2:C:15:LEU:CD2   | 0.55     | 2.69        | 5      | 2     |
| 1:A:506:LEU:C    | 1:A:508:LEU:H    | 0.55     | 2.08        | 3      | 6     |
| 2:C:8:LEU:C      | 2:C:9:THR:HG22   | 0.55     | 2.26        | 2      | 1     |
| 1:A:593:HIS:O    | 1:A:595:MET:N    | 0.55     | 2.40        | 3      | 2     |
| 1:A:552:GLU:O    | 1:A:553:ARG:C    | 0.55     | 2.50        | 6      | 2     |
| 1:A:506:LEU:C    | 1:A:508:LEU:N    | 0.55     | 2.65        | 5      | 7     |
| 1:A:583:ASP:OD1  | 2:B:68:HIS:NE2   | 0.55     | 2.40        | 7      | 3     |
| 2:B:58:ASP:OD1   | 2:B:58:ASP:N     | 0.55     | 2.40        | 9      | 1     |
| 1:A:530:LEU:C    | 1:A:530:LEU:HD23 | 0.55     | 2.26        | 8      | 2     |
| 1:A:497:PHE:O    | 1:A:497:PHE:CG   | 0.55     | 2.60        | 9      | 1     |
| 1:A:493:LEU:O    | 1:A:497:PHE:CD1  | 0.54     | 2.59        | 10     | 3     |
| 1:A:515:SER:C    | 1:A:516:THR:OG1  | 0.54     | 2.50        | 8      | 4     |
| 2:B:58:ASP:O     | 2:B:59:TYR:CD1   | 0.54     | 2.60        | 3      | 1     |
| 2:C:44:ILE:HD12  | 2:C:70:VAL:CG2   | 0.54     | 2.29        | 3      | 2     |
| 2:B:22:THR:OG1   | 2:B:25:ASN:ND2   | 0.54     | 2.40        | 10     | 1     |
| 2:C:7:THR:O      | 2:C:9:THR:N      | 0.54     | 2.40        | 2      | 4     |
| 1:A:510:LEU:CB   | 1:A:511:PRO:CD   | 0.54     | 2.86        | 4      | 10    |
| 1:A:493:LEU:O    | 1:A:497:PHE:CE2  | 0.54     | 2.61        | 7      | 4     |
| 2:C:18:GLU:N     | 2:C:21:ASP:OD2   | 0.54     | 2.41        | 5      | 2     |
| 2:C:45:PHE:CD2   | 2:C:46:ALA:N     | 0.54     | 2.75        | 8      | 2     |
| 1:A:530:LEU:HD23 | 1:A:530:LEU:O    | 0.54     | 2.02        | 3      | 5     |
| 1:A:548:ASP:CG   | 2:B:71:LEU:O     | 0.54     | 2.51        | 9      | 4     |
| 2:B:38:PRO:C     | 2:B:40:GLN:N     | 0.54     | 2.66        | 3      | 9     |
| 1:A:504:GLU:OE2  | 2:C:6:LYS:NZ     | 0.54     | 2.41        | 6      | 2     |
| 2:C:38:PRO:O     | 2:C:40:GLN:N     | 0.54     | 2.41        | 6      | 5     |
| 2:B:76:GLY:OXT   | 2:C:68:HIS:CG    | 0.54     | 2.61        | 9      | 1     |
| 2:B:25:ASN:HD22  | 2:B:25:ASN:N     | 0.54     | 1.98        | 10     | 1     |
| 2:B:67:LEU:CD1   | 2:B:67:LEU:N     | 0.53     | 2.70        | 2      | 1     |
| 2:B:69:LEU:C     | 2:B:69:LEU:CD2   | 0.53     | 2.81        | 4      | 3     |
| 2:C:42:ARG:NE    | 2:C:49:GLN:CD    | 0.53     | 2.66        | 3      | 2     |
| 2:C:71:LEU:HD12  | 2:C:71:LEU:N     | 0.53     | 2.18        | 4      | 1     |
| 1:A:525:MET:SD   | 1:A:525:MET:N    | 0.53     | 2.81        | 7      | 1     |
| 1:A:518:LEU:O    | 1:A:519:PRO:O    | 0.53     | 2.25        | 6      | 6     |
| 1:A:551:LEU:CD1  | 1:A:551:LEU:N    | 0.53     | 2.71        | 4      | 2     |
| 1:A:593:HIS:N    | 1:A:594:PRO:CD   | 0.53     | 2.70        | 6      | 3     |
| 2:C:45:PHE:O     | 2:C:47:GLY:N     | 0.53     | 2.41        | 8      | 1     |
| 2:C:7:THR:OG1    | 2:C:10:GLY:CA    | 0.53     | 2.56        | 6      | 4     |
| 2:C:38:PRO:C     | 2:C:40:GLN:N     | 0.53     | 2.67        | 5      | 6     |
| 2:B:45:PHE:C     | 2:B:47:GLY:N     | 0.53     | 2.66        | 8      | 5     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:580:GLN:CD   | 1:A:580:GLN:N    | 0.53     | 2.66        | 4      | 1     |
| 1:A:556:ILE:C    | 1:A:558:LEU:N    | 0.53     | 2.67        | 1      | 4     |
| 1:A:517:ASP:CG   | 2:C:72:ARG:NH1   | 0.53     | 2.67        | 8      | 1     |
| 1:A:514:ALA:HB1  | 2:B:73:LEU:HD12  | 0.53     | 1.80        | 6      | 2     |
| 1:A:552:GLU:CD   | 2:B:42:ARG:HH22  | 0.53     | 2.12        | 5      | 1     |
| 2:C:42:ARG:NE    | 2:C:49:GLN:OE1   | 0.53     | 2.42        | 4      | 2     |
| 2:B:71:LEU:O     | 2:B:72:ARG:O     | 0.53     | 2.26        | 9      | 3     |
| 2:C:17:VAL:HG21  | 2:C:56:LEU:CD1   | 0.53     | 2.34        | 6      | 5     |
| 1:A:515:SER:C    | 1:A:516:THR:HG1  | 0.53     | 2.12        | 9      | 2     |
| 1:A:552:GLU:HG3  | 1:A:554:THR:OG1  | 0.53     | 2.04        | 8      | 1     |
| 1:A:491:LEU:C    | 1:A:491:LEU:HD23 | 0.52     | 2.28        | 7      | 4     |
| 1:A:595:MET:C    | 1:A:597:SER:N    | 0.52     | 2.66        | 4      | 3     |
| 1:A:511:PRO:C    | 1:A:513:ALA:N    | 0.52     | 2.65        | 10     | 3     |
| 1:A:497:PHE:C    | 1:A:499:GLY:H    | 0.52     | 2.12        | 10     | 2     |
| 2:B:71:LEU:HD23  | 2:B:71:LEU:H     | 0.52     | 1.64        | 9      | 1     |
| 2:B:1:MET:HE2    | 2:B:19:PRO:HG3   | 0.52     | 1.80        | 1      | 1     |
| 1:A:509:LEU:HD23 | 1:A:509:LEU:O    | 0.52     | 2.04        | 8      | 2     |
| 1:A:583:ASP:OD2  | 2:B:68:HIS:NE2   | 0.52     | 2.42        | 10     | 2     |
| 1:A:514:ALA:C    | 1:A:516:THR:N    | 0.52     | 2.66        | 10     | 1     |
| 2:B:1:MET:N      | 2:B:18:GLU:OE2   | 0.52     | 2.43        | 10     | 1     |
| 2:C:20:SER:O     | 2:C:21:ASP:C     | 0.52     | 2.53        | 5      | 1     |
| 1:A:587:THR:O    | 1:A:590:ALA:N    | 0.52     | 2.42        | 7      | 5     |
| 1:A:544:THR:O    | 1:A:548:ASP:OD2  | 0.52     | 2.28        | 9      | 1     |
| 2:C:42:ARG:HE    | 2:C:49:GLN:CD    | 0.52     | 2.13        | 3      | 2     |
| 1:A:552:GLU:OE2  | 2:B:42:ARG:NH2   | 0.52     | 2.43        | 9      | 2     |
| 2:C:18:GLU:H     | 2:C:21:ASP:CG    | 0.52     | 2.13        | 3      | 4     |
| 1:A:549:ASN:O    | 1:A:553:ARG:CA   | 0.51     | 2.57        | 4      | 4     |
| 1:A:552:GLU:O    | 1:A:554:THR:N    | 0.51     | 2.43        | 7      | 3     |
| 1:A:582:ASP:N    | 1:A:582:ASP:OD1  | 0.51     | 2.42        | 1      | 2     |
| 1:A:497:PHE:C    | 1:A:499:GLY:N    | 0.51     | 2.67        | 4      | 3     |
| 1:A:594:PRO:C    | 1:A:596:THR:N    | 0.51     | 2.67        | 4      | 2     |
| 2:B:14:THR:C     | 2:B:15:LEU:HD22  | 0.51     | 2.30        | 10     | 1     |
| 2:B:67:LEU:N     | 2:B:67:LEU:HD12  | 0.51     | 2.19        | 2      | 1     |
| 2:B:7:THR:C      | 2:B:9:THR:N      | 0.51     | 2.67        | 9      | 5     |
| 2:B:18:GLU:O     | 2:B:20:SER:N     | 0.51     | 2.42        | 3      | 1     |
| 2:B:58:ASP:C     | 2:B:59:TYR:CD1   | 0.51     | 2.88        | 3      | 2     |
| 2:C:5:VAL:N      | 2:C:13:ILE:O     | 0.51     | 2.43        | 9      | 5     |
| 2:B:19:PRO:O     | 2:B:57:SER:OG    | 0.51     | 2.27        | 1      | 2     |
| 2:C:1:MET:N      | 2:C:17:VAL:O     | 0.51     | 2.38        | 2      | 7     |
| 1:A:571:GLY:C    | 1:A:573:LEU:N    | 0.51     | 2.68        | 9      | 2     |
| 2:B:27:LYS:NZ    | 2:B:41:GLN:O     | 0.51     | 2.44        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:510:LEU:O    | 1:A:513:ALA:HB3  | 0.51     | 2.06        | 5      | 4     |
| 2:B:52:ASP:OD1   | 2:B:52:ASP:N     | 0.51     | 2.44        | 2      | 1     |
| 2:B:71:LEU:N     | 2:B:71:LEU:CD1   | 0.51     | 2.74        | 3      | 1     |
| 1:A:593:HIS:O    | 1:A:593:HIS:CG   | 0.51     | 2.62        | 5      | 1     |
| 2:B:4:PHE:CE2    | 2:B:14:THR:OG1   | 0.51     | 2.60        | 7      | 1     |
| 2:C:58:ASP:N     | 2:C:58:ASP:OD1   | 0.51     | 2.42        | 4      | 1     |
| 1:A:539:ASN:OD1  | 1:A:540:GLY:N    | 0.51     | 2.43        | 9      | 1     |
| 1:A:537:THR:OG1  | 1:A:538:CYS:N    | 0.51     | 2.43        | 5      | 2     |
| 1:A:521:GLU:C    | 1:A:523:ALA:N    | 0.50     | 2.68        | 1      | 1     |
| 2:B:54:ARG:N     | 2:B:54:ARG:NE    | 0.50     | 2.58        | 2      | 1     |
| 2:C:25:ASN:OD1   | 2:C:29:LYS:NZ    | 0.50     | 2.44        | 4      | 1     |
| 1:A:506:LEU:HD12 | 1:A:506:LEU:N    | 0.50     | 2.21        | 6      | 2     |
| 1:A:593:HIS:C    | 1:A:595:MET:N    | 0.50     | 2.69        | 3      | 2     |
| 1:A:577:GLN:N    | 1:A:577:GLN:CD   | 0.50     | 2.69        | 8      | 2     |
| 1:A:602:LEU:CD2  | 1:A:602:LEU:N    | 0.50     | 2.73        | 8      | 1     |
| 1:A:583:ASP:CG   | 2:B:68:HIS:NE2   | 0.50     | 2.69        | 2      | 2     |
| 1:A:549:ASN:C    | 1:A:551:LEU:N    | 0.50     | 2.67        | 7      | 2     |
| 1:A:602:LEU:C    | 1:A:602:LEU:HD23 | 0.50     | 2.31        | 3      | 5     |
| 1:A:549:ASN:O    | 1:A:551:LEU:N    | 0.50     | 2.45        | 7      | 1     |
| 2:C:15:LEU:HD12  | 2:C:15:LEU:N     | 0.50     | 2.21        | 2      | 2     |
| 1:A:593:HIS:O    | 1:A:593:HIS:ND1  | 0.50     | 2.44        | 4      | 1     |
| 1:A:602:LEU:N    | 1:A:602:LEU:HD22 | 0.50     | 2.21        | 8      | 1     |
| 1:A:575:MET:SD   | 1:A:575:MET:C    | 0.50     | 2.95        | 3      | 1     |
| 2:C:51:GLU:N     | 2:C:51:GLU:CD    | 0.50     | 2.69        | 10     | 1     |
| 1:A:493:LEU:O    | 1:A:497:PHE:CE1  | 0.50     | 2.65        | 10     | 2     |
| 1:A:569:ALA:C    | 1:A:571:GLY:N    | 0.50     | 2.68        | 10     | 4     |
| 1:A:553:ARG:C    | 1:A:554:THR:OG1  | 0.50     | 2.54        | 9      | 2     |
| 1:A:583:ASP:O    | 1:A:586:GLU:N    | 0.50     | 2.45        | 2      | 2     |
| 2:C:31:GLN:OE1   | 2:C:36:ILE:C     | 0.50     | 2.55        | 2      | 1     |
| 1:A:591:ILE:HD12 | 1:A:591:ILE:N    | 0.50     | 2.22        | 5      | 1     |
| 2:B:44:ILE:CG2   | 2:B:45:PHE:N     | 0.50     | 2.75        | 7      | 2     |
| 1:A:581:VAL:HG13 | 1:A:582:ASP:N    | 0.49     | 2.21        | 1      | 1     |
| 2:C:21:ASP:OD1   | 2:C:21:ASP:N     | 0.49     | 2.43        | 5      | 1     |
| 1:A:495:ILE:C    | 1:A:495:ILE:CD1  | 0.49     | 2.85        | 10     | 1     |
| 1:A:517:ASP:O    | 1:A:518:LEU:C    | 0.49     | 2.54        | 1      | 3     |
| 1:A:517:ASP:CG   | 1:A:518:LEU:N    | 0.49     | 2.71        | 5      | 2     |
| 2:C:11:LYS:HG3   | 2:C:12:THR:N     | 0.49     | 2.22        | 1      | 5     |
| 2:C:7:THR:C      | 2:C:9:THR:N      | 0.49     | 2.69        | 2      | 3     |
| 1:A:578:GLY:C    | 1:A:580:GLN:H    | 0.49     | 2.12        | 5      | 2     |
| 2:B:44:ILE:HG22  | 2:B:45:PHE:N     | 0.49     | 2.20        | 7      | 1     |
| 1:A:583:ASP:OD2  | 2:B:6:LYS:NZ     | 0.49     | 2.42        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:C:58:ASP:O     | 2:C:59:TYR:CD2   | 0.49     | 2.66        | 5      | 1     |
| 1:A:516:THR:C    | 1:A:517:ASP:CG   | 0.49     | 2.80        | 6      | 1     |
| 1:A:547:MET:C    | 1:A:549:ASN:N    | 0.49     | 2.70        | 1      | 2     |
| 2:C:60:ASN:N     | 2:C:60:ASN:ND2   | 0.49     | 2.61        | 5      | 1     |
| 1:A:502:ASN:C    | 1:A:504:GLU:N    | 0.49     | 2.70        | 7      | 1     |
| 1:A:528:LEU:C    | 1:A:528:LEU:HD23 | 0.49     | 2.33        | 5      | 4     |
| 1:A:593:HIS:C    | 1:A:595:MET:H    | 0.49     | 2.16        | 3      | 2     |
| 2:B:46:ALA:O     | 2:B:47:GLY:C     | 0.49     | 2.56        | 2      | 1     |
| 2:B:18:GLU:C     | 2:B:20:SER:N     | 0.49     | 2.71        | 3      | 1     |
| 1:A:515:SER:O    | 1:A:515:SER:OG   | 0.49     | 2.31        | 5      | 1     |
| 1:A:546:ILE:HG22 | 1:A:547:MET:N    | 0.49     | 2.23        | 6      | 2     |
| 1:A:552:GLU:O    | 1:A:553:ARG:HB2  | 0.49     | 2.07        | 5      | 1     |
| 1:A:571:GLY:O    | 1:A:573:LEU:N    | 0.49     | 2.45        | 9      | 1     |
| 1:A:503:ASP:OD1  | 1:A:503:ASP:N    | 0.49     | 2.45        | 10     | 1     |
| 1:A:521:GLU:C    | 1:A:523:ALA:H    | 0.49     | 2.16        | 1      | 1     |
| 2:B:38:PRO:O     | 2:B:40:GLN:N     | 0.49     | 2.45        | 8      | 7     |
| 1:A:502:ASN:C    | 1:A:504:GLU:H    | 0.49     | 2.15        | 7      | 1     |
| 1:A:549:ASN:C    | 1:A:549:ASN:HD22 | 0.49     | 2.16        | 8      | 1     |
| 2:C:60:ASN:N     | 2:C:60:ASN:HD22  | 0.49     | 2.06        | 5      | 1     |
| 2:B:39:ASP:N     | 2:B:39:ASP:OD1   | 0.48     | 2.46        | 5      | 2     |
| 2:B:73:LEU:CD2   | 2:B:73:LEU:H     | 0.48     | 2.21        | 10     | 1     |
| 2:B:25:ASN:OD1   | 2:B:29:LYS:NZ    | 0.48     | 2.42        | 2      | 1     |
| 1:A:493:LEU:O    | 1:A:496:ALA:HB3  | 0.48     | 2.08        | 6      | 1     |
| 1:A:520:ILE:CD1  | 1:A:555:ALA:O    | 0.48     | 2.61        | 7      | 2     |
| 1:A:548:ASP:OD2  | 2:B:72:ARG:C     | 0.48     | 2.56        | 7      | 2     |
| 1:A:556:ILE:HD11 | 1:A:562:TRP:CZ2  | 0.48     | 2.42        | 10     | 1     |
| 1:A:552:GLU:OE2  | 2:B:42:ARG:CZ    | 0.48     | 2.62        | 1      | 1     |
| 2:B:45:PHE:O     | 2:B:46:ALA:C     | 0.48     | 2.56        | 7      | 8     |
| 1:A:548:ASP:OD1  | 2:B:71:LEU:O     | 0.48     | 2.31        | 6      | 3     |
| 1:A:559:LYS:C    | 1:A:560:THR:HG1  | 0.48     | 2.14        | 6      | 1     |
| 2:B:7:THR:C      | 2:B:9:THR:H      | 0.48     | 2.17        | 6      | 6     |
| 1:A:595:MET:O    | 1:A:597:SER:N    | 0.48     | 2.47        | 4      | 1     |
| 2:B:7:THR:O      | 2:B:9:THR:N      | 0.48     | 2.46        | 9      | 2     |
| 2:B:19:PRO:C     | 2:B:57:SER:HG    | 0.48     | 2.16        | 1      | 1     |
| 2:C:18:GLU:O     | 2:C:20:SER:N     | 0.48     | 2.46        | 3      | 1     |
| 1:A:501:LYS:CD   | 1:A:501:LYS:N    | 0.48     | 2.77        | 6      | 1     |
| 2:B:17:VAL:HG21  | 2:B:56:LEU:CD1   | 0.48     | 2.39        | 4      | 2     |
| 2:B:72:ARG:O     | 2:B:74:ARG:N     | 0.48     | 2.46        | 5      | 2     |
| 1:A:509:LEU:C    | 1:A:509:LEU:CD1  | 0.48     | 2.87        | 10     | 1     |
| 1:A:511:PRO:O    | 1:A:515:SER:CB   | 0.48     | 2.61        | 1      | 1     |
| 2:B:18:GLU:CB    | 2:B:19:PRO:CD    | 0.48     | 2.91        | 1      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:B:22:THR:O     | 2:B:25:ASN:N     | 0.48     | 2.46        | 5      | 4     |
| 2:B:72:ARG:CG    | 2:B:73:LEU:N     | 0.48     | 2.77        | 3      | 2     |
| 2:C:8:LEU:O      | 2:C:9:THR:CG2    | 0.48     | 2.59        | 9      | 6     |
| 1:A:541:ASP:O    | 1:A:544:THR:OG1  | 0.48     | 2.31        | 3      | 3     |
| 2:C:52:ASP:OD1   | 2:C:52:ASP:N     | 0.48     | 2.46        | 10     | 2     |
| 2:C:8:LEU:C      | 2:C:9:THR:OG1    | 0.48     | 2.54        | 8      | 1     |
| 1:A:590:ALA:O    | 2:B:47:GLY:O     | 0.48     | 2.31        | 9      | 1     |
| 1:A:535:VAL:HG13 | 1:A:536:GLY:N    | 0.48     | 2.24        | 10     | 5     |
| 1:A:540:GLY:C    | 1:A:542:ILE:N    | 0.48     | 2.71        | 2      | 3     |
| 2:C:71:LEU:N     | 2:C:71:LEU:CD1   | 0.48     | 2.77        | 4      | 1     |
| 2:B:18:GLU:O     | 2:B:21:ASP:N     | 0.47     | 2.47        | 6      | 4     |
| 2:C:1:MET:HE1    | 2:C:61:ILE:O     | 0.47     | 2.09        | 10     | 2     |
| 1:A:514:ALA:CB   | 2:B:73:LEU:HD12  | 0.47     | 2.38        | 6      | 1     |
| 1:A:562:TRP:C    | 1:A:564:ARG:N    | 0.47     | 2.72        | 8      | 1     |
| 1:A:507:GLY:O    | 1:A:511:PRO:CG   | 0.47     | 2.62        | 10     | 1     |
| 1:A:542:ILE:C    | 1:A:544:THR:N    | 0.47     | 2.70        | 9      | 3     |
| 2:B:14:THR:C     | 2:B:15:LEU:HD12  | 0.47     | 2.33        | 1      | 1     |
| 2:C:8:LEU:HD11   | 2:C:70:VAL:HG13  | 0.47     | 1.86        | 4      | 1     |
| 2:C:59:TYR:C     | 2:C:60:ASN:HD22  | 0.47     | 2.17        | 5      | 1     |
| 1:A:544:THR:O    | 1:A:548:ASP:OD1  | 0.47     | 2.31        | 6      | 1     |
| 2:B:45:PHE:O     | 2:B:48:LYS:N     | 0.47     | 2.48        | 8      | 1     |
| 1:A:538:CYS:SG   | 1:A:573:LEU:O    | 0.47     | 2.73        | 3      | 1     |
| 2:C:9:THR:OG1    | 2:C:9:THR:O      | 0.47     | 2.32        | 5      | 1     |
| 1:A:556:ILE:C    | 1:A:558:LEU:H    | 0.47     | 2.18        | 7      | 2     |
| 1:A:509:LEU:O    | 1:A:509:LEU:HD13 | 0.47     | 2.09        | 10     | 1     |
| 1:A:511:PRO:O    | 1:A:515:SER:OG   | 0.47     | 2.31        | 1      | 1     |
| 2:B:38:PRO:O     | 2:B:39:ASP:C     | 0.47     | 2.58        | 8      | 2     |
| 1:A:515:SER:O    | 2:C:42:ARG:NH2   | 0.47     | 2.46        | 9      | 1     |
| 2:B:53:GLY:O     | 2:B:54:ARG:O     | 0.47     | 2.33        | 9      | 9     |
| 1:A:540:GLY:O    | 1:A:541:ASP:C    | 0.47     | 2.58        | 9      | 6     |
| 2:B:54:ARG:NE    | 2:B:54:ARG:CA    | 0.47     | 2.78        | 2      | 1     |
| 1:A:594:PRO:O    | 1:A:596:THR:N    | 0.47     | 2.47        | 4      | 1     |
| 2:B:74:ARG:NH2   | 2:C:47:GLY:CA    | 0.47     | 2.78        | 4      | 1     |
| 1:A:540:GLY:O    | 1:A:544:THR:HG23 | 0.47     | 2.10        | 7      | 1     |
| 1:A:552:GLU:O    | 1:A:553:ARG:CB   | 0.47     | 2.61        | 8      | 1     |
| 2:C:18:GLU:C     | 2:C:20:SER:N     | 0.47     | 2.73        | 3      | 1     |
| 2:B:72:ARG:O     | 2:B:73:LEU:C     | 0.47     | 2.58        | 9      | 2     |
| 1:A:493:LEU:HD12 | 1:A:493:LEU:N    | 0.47     | 2.25        | 8      | 2     |
| 1:A:497:PHE:O    | 1:A:498:ALA:C    | 0.47     | 2.57        | 6      | 2     |
| 1:A:544:THR:O    | 1:A:548:ASP:CG   | 0.47     | 2.58        | 1      | 1     |
| 2:C:57:SER:C     | 2:C:59:TYR:H     | 0.47     | 2.18        | 5      | 3     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:587:THR:O    | 1:A:590:ALA:HB3  | 0.47     | 2.10        | 4      | 2     |
| 1:A:515:SER:OG   | 1:A:518:LEU:CD1  | 0.47     | 2.63        | 9      | 1     |
| 1:A:509:LEU:C    | 1:A:509:LEU:HD13 | 0.47     | 2.35        | 10     | 1     |
| 2:B:51:GLU:N     | 2:B:51:GLU:CD    | 0.47     | 2.73        | 10     | 1     |
| 1:A:509:LEU:C    | 1:A:509:LEU:CD2  | 0.46     | 2.88        | 2      | 2     |
| 1:A:510:LEU:O    | 1:A:514:ALA:N    | 0.46     | 2.47        | 4      | 1     |
| 2:C:58:ASP:C     | 2:C:59:TYR:CD2   | 0.46     | 2.93        | 5      | 1     |
| 1:A:515:SER:OG   | 1:A:517:ASP:OD1  | 0.46     | 2.33        | 7      | 1     |
| 1:A:505:VAL:O    | 1:A:509:LEU:CB   | 0.46     | 2.63        | 9      | 2     |
| 1:A:520:ILE:HD12 | 1:A:558:LEU:O    | 0.46     | 2.10        | 9      | 2     |
| 1:A:606:CYS:O    | 1:A:607:ALA:HB2  | 0.46     | 2.10        | 2      | 1     |
| 1:A:533:VAL:C    | 1:A:535:VAL:H    | 0.46     | 2.19        | 3      | 7     |
| 2:B:55:THR:OG1   | 2:B:57:SER:OG    | 0.46     | 2.32        | 5      | 2     |
| 1:A:548:ASP:O    | 1:A:552:GLU:N    | 0.46     | 2.48        | 6      | 1     |
| 1:A:540:GLY:O    | 1:A:542:ILE:N    | 0.46     | 2.48        | 2      | 3     |
| 1:A:548:ASP:OD2  | 2:B:71:LEU:O     | 0.46     | 2.33        | 2      | 2     |
| 1:A:591:ILE:O    | 1:A:592:GLU:O    | 0.46     | 2.33        | 9      | 4     |
| 1:A:595:MET:C    | 1:A:597:SER:H    | 0.46     | 2.17        | 4      | 1     |
| 2:C:45:PHE:O     | 2:C:46:ALA:C     | 0.46     | 2.59        | 5      | 2     |
| 1:A:517:ASP:O    | 1:A:518:LEU:O    | 0.46     | 2.33        | 1      | 4     |
| 1:A:552:GLU:CG   | 2:B:42:ARG:HH12  | 0.46     | 2.23        | 5      | 3     |
| 1:A:506:LEU:N    | 1:A:506:LEU:CD1  | 0.46     | 2.79        | 2      | 2     |
| 2:B:18:GLU:C     | 2:B:20:SER:H     | 0.46     | 2.18        | 3      | 1     |
| 1:A:542:ILE:O    | 1:A:543:THR:C    | 0.46     | 2.59        | 7      | 2     |
| 1:A:491:LEU:C    | 1:A:491:LEU:CD2  | 0.46     | 2.88        | 7      | 4     |
| 2:C:22:THR:O     | 2:C:23:ILE:C     | 0.46     | 2.59        | 10     | 2     |
| 2:C:14:THR:C     | 2:C:15:LEU:HD22  | 0.46     | 2.34        | 6      | 2     |
| 1:A:516:THR:C    | 1:A:517:ASP:OD1  | 0.46     | 2.58        | 7      | 1     |
| 2:B:45:PHE:C     | 2:B:47:GLY:H     | 0.46     | 2.18        | 8      | 1     |
| 2:B:2:GLN:O      | 2:B:64:GLU:OE2   | 0.46     | 2.34        | 10     | 1     |
| 1:A:581:VAL:CG1  | 1:A:582:ASP:N    | 0.46     | 2.79        | 1      | 1     |
| 2:C:18:GLU:CB    | 2:C:19:PRO:CD    | 0.46     | 2.93        | 1      | 3     |
| 1:A:568:LEU:C    | 1:A:568:LEU:HD23 | 0.46     | 2.35        | 2      | 1     |
| 1:A:551:LEU:HD22 | 2:B:42:ARG:NH2   | 0.46     | 2.26        | 4      | 1     |
| 1:A:497:PHE:CD2  | 1:A:505:VAL:HG21 | 0.46     | 2.46        | 10     | 1     |
| 1:A:569:ALA:C    | 1:A:571:GLY:H    | 0.46     | 2.19        | 10     | 1     |
| 1:A:539:ASN:CG   | 1:A:540:GLY:H    | 0.46     | 2.18        | 9      | 2     |
| 1:A:509:LEU:HD23 | 1:A:509:LEU:C    | 0.46     | 2.35        | 8      | 1     |
| 1:A:530:LEU:C    | 1:A:530:LEU:CD2  | 0.46     | 2.89        | 8      | 2     |
| 1:A:547:MET:C    | 1:A:549:ASN:H    | 0.46     | 2.19        | 1      | 1     |
| 1:A:497:PHE:O    | 1:A:499:GLY:N    | 0.46     | 2.49        | 4      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 2:C:53:GLY:O     | 2:C:54:ARG:O     | 0.45     | 2.33        | 8      | 4     |
| 1:A:507:GLY:O    | 1:A:511:PRO:CD   | 0.45     | 2.64        | 10     | 1     |
| 1:A:549:ASN:O    | 1:A:553:ARG:HA   | 0.45     | 2.12        | 7      | 2     |
| 1:A:580:GLN:H    | 1:A:580:GLN:NE2  | 0.45     | 2.08        | 4      | 1     |
| 1:A:539:ASN:CG   | 1:A:540:GLY:N    | 0.45     | 2.74        | 9      | 1     |
| 1:A:559:LYS:O    | 1:A:560:THR:OG1  | 0.45     | 2.35        | 9      | 4     |
| 2:B:1:MET:SD     | 2:B:17:VAL:HG23  | 0.45     | 2.51        | 3      | 1     |
| 2:C:25:ASN:HD22  | 2:C:25:ASN:C     | 0.45     | 2.20        | 2      | 2     |
| 1:A:528:LEU:C    | 1:A:528:LEU:CD2  | 0.45     | 2.90        | 8      | 4     |
| 2:C:22:THR:OG1   | 2:C:25:ASN:OD1   | 0.45     | 2.35        | 3      | 2     |
| 2:B:57:SER:C     | 2:B:59:TYR:H     | 0.45     | 2.19        | 9      | 2     |
| 2:B:16:GLU:CD    | 2:B:16:GLU:N     | 0.45     | 2.75        | 7      | 1     |
| 1:A:594:PRO:C    | 1:A:596:THR:H    | 0.45     | 2.20        | 4      | 1     |
| 1:A:602:LEU:C    | 1:A:602:LEU:CD2  | 0.45     | 2.89        | 9      | 5     |
| 2:B:23:ILE:HG22  | 2:B:27:LYS:NZ    | 0.45     | 2.25        | 2      | 1     |
| 1:A:506:LEU:CD2  | 1:A:530:LEU:HD21 | 0.45     | 2.42        | 8      | 1     |
| 1:A:600:GLU:CD   | 1:A:600:GLU:C    | 0.45     | 2.84        | 2      | 2     |
| 2:B:17:VAL:C     | 2:B:18:GLU:CD    | 0.45     | 2.85        | 8      | 1     |
| 2:B:22:THR:O     | 2:B:23:ILE:C     | 0.45     | 2.59        | 5      | 4     |
| 1:A:531:ALA:O    | 1:A:535:VAL:N    | 0.45     | 2.50        | 8      | 6     |
| 1:A:558:LEU:HD23 | 1:A:558:LEU:N    | 0.45     | 2.27        | 7      | 1     |
| 1:A:569:ALA:O    | 1:A:573:LEU:N    | 0.45     | 2.50        | 1      | 2     |
| 1:A:591:ILE:O    | 1:A:592:GLU:C    | 0.45     | 2.58        | 5      | 1     |
| 1:A:520:ILE:CG2  | 1:A:555:ALA:HB1  | 0.45     | 2.43        | 6      | 1     |
| 2:C:59:TYR:C     | 2:C:60:ASN:CG    | 0.45     | 2.85        | 9      | 1     |
| 1:A:541:ASP:CG   | 2:B:74:ARG:HH22  | 0.44     | 2.20        | 2      | 1     |
| 1:A:558:LEU:C    | 1:A:558:LEU:HD23 | 0.44     | 2.36        | 5      | 1     |
| 2:B:32:ASP:OD1   | 2:B:32:ASP:O     | 0.44     | 2.35        | 3      | 2     |
| 2:C:55:THR:C     | 2:C:57:SER:H     | 0.44     | 2.19        | 7      | 2     |
| 1:A:538:CYS:O    | 1:A:538:CYS:SG   | 0.44     | 2.74        | 1      | 1     |
| 2:C:16:GLU:CD    | 2:C:16:GLU:C     | 0.44     | 2.85        | 5      | 1     |
| 2:C:16:GLU:CD    | 2:C:16:GLU:O     | 0.44     | 2.60        | 5      | 1     |
| 1:A:551:LEU:O    | 1:A:552:GLU:C    | 0.44     | 2.60        | 6      | 2     |
| 2:B:59:TYR:O     | 2:B:60:ASN:CG    | 0.44     | 2.60        | 1      | 1     |
| 2:C:59:TYR:O     | 2:C:60:ASN:CG    | 0.44     | 2.60        | 2      | 2     |
| 1:A:560:THR:OG1  | 1:A:561:ASP:N    | 0.44     | 2.50        | 7      | 1     |
| 1:A:596:THR:O    | 1:A:597:SER:C    | 0.44     | 2.60        | 9      | 3     |
| 1:A:506:LEU:O    | 1:A:507:GLY:C    | 0.44     | 2.60        | 9      | 2     |
| 1:A:514:ALA:O    | 1:A:516:THR:N    | 0.44     | 2.51        | 10     | 1     |
| 1:A:502:ASN:CG   | 1:A:503:ASP:H    | 0.44     | 2.20        | 5      | 1     |
| 1:A:580:GLN:CD   | 1:A:580:GLN:C    | 0.44     | 2.86        | 10     | 1     |

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| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:549:ASN:O    | 1:A:550:PHE:C   | 0.44     | 2.60        | 2      | 5     |
| 1:A:550:PHE:CZ   | 1:A:566:LEU:CD2 | 0.44     | 3.01        | 9      | 1     |
| 1:A:517:ASP:OD2  | 1:A:518:LEU:N   | 0.44     | 2.51        | 1      | 1     |
| 1:A:583:ASP:O    | 1:A:584:VAL:C   | 0.44     | 2.61        | 2      | 1     |
| 1:A:558:LEU:C    | 1:A:558:LEU:CD2 | 0.44     | 2.91        | 5      | 1     |
| 1:A:543:THR:O    | 1:A:545:SER:N   | 0.44     | 2.51        | 6      | 1     |
| 1:A:538:CYS:O    | 1:A:539:ASN:OD1 | 0.44     | 2.36        | 8      | 1     |
| 1:A:562:TRP:CD1  | 1:A:562:TRP:N   | 0.44     | 2.85        | 8      | 1     |
| 1:A:574:TYR:CZ   | 1:A:580:GLN:NE2 | 0.44     | 2.85        | 10     | 1     |
| 2:B:24:GLU:CD    | 2:B:24:GLU:C    | 0.44     | 2.85        | 8      | 1     |
| 1:A:504:GLU:O    | 1:A:505:VAL:C   | 0.43     | 2.61        | 9      | 6     |
| 2:C:25:ASN:O     | 2:C:28:ALA:HB3  | 0.43     | 2.13        | 5      | 2     |
| 2:B:69:LEU:HD21  | 2:B:71:LEU:CD1  | 0.43     | 2.43        | 6      | 1     |
| 1:A:576:GLY:O    | 1:A:577:GLN:O   | 0.43     | 2.36        | 7      | 2     |
| 1:A:506:LEU:O    | 1:A:510:LEU:HB3 | 0.43     | 2.12        | 10     | 1     |
| 1:A:552:GLU:O    | 1:A:553:ARG:O   | 0.43     | 2.36        | 6      | 1     |
| 1:A:508:LEU:HD11 | 2:C:8:LEU:O     | 0.43     | 2.13        | 2      | 1     |
| 1:A:528:LEU:O    | 1:A:531:ALA:N   | 0.43     | 2.48        | 4      | 2     |
| 1:A:569:ALA:O    | 1:A:571:GLY:N   | 0.43     | 2.51        | 10     | 3     |
| 1:A:556:ILE:O    | 1:A:558:LEU:CD2 | 0.43     | 2.65        | 7      | 1     |
| 1:A:498:ALA:O    | 1:A:499:GLY:O   | 0.43     | 2.35        | 10     | 1     |
| 2:B:19:PRO:C     | 2:B:57:SER:OG   | 0.43     | 2.61        | 1      | 1     |
| 2:C:18:GLU:C     | 2:C:20:SER:H    | 0.43     | 2.21        | 3      | 1     |
| 2:C:24:GLU:CD    | 2:C:24:GLU:C    | 0.43     | 2.85        | 4      | 1     |
| 1:A:515:SER:O    | 1:A:516:THR:OG1 | 0.43     | 2.35        | 9      | 3     |
| 1:A:541:ASP:OD1  | 2:B:74:ARG:CZ   | 0.43     | 2.67        | 10     | 1     |
| 1:A:592:GLU:O    | 1:A:593:HIS:C   | 0.43     | 2.62        | 3      | 2     |
| 1:A:586:GLU:CD   | 1:A:586:GLU:C   | 0.43     | 2.85        | 5      | 1     |
| 1:A:516:THR:O    | 1:A:517:ASP:CG  | 0.43     | 2.61        | 6      | 1     |
| 1:A:542:ILE:O    | 1:A:544:THR:N   | 0.43     | 2.52        | 9      | 3     |
| 2:B:15:LEU:HD12  | 2:B:15:LEU:N    | 0.43     | 2.28        | 1      | 1     |
| 2:B:71:LEU:O     | 2:B:72:ARG:C    | 0.43     | 2.60        | 9      | 1     |
| 1:A:486:SER:OG   | 1:A:487:SER:N   | 0.43     | 2.51        | 1      | 2     |
| 2:C:55:THR:OG1   | 2:C:57:SER:OG   | 0.43     | 2.35        | 9      | 1     |
| 1:A:510:LEU:HB3  | 1:A:511:PRO:HD3 | 0.43     | 1.91        | 10     | 1     |
| 1:A:516:THR:O    | 1:A:517:ASP:CB  | 0.43     | 2.66        | 10     | 1     |
| 1:A:574:TYR:CE2  | 1:A:580:GLN:NE2 | 0.43     | 2.86        | 10     | 1     |
| 1:A:572:ILE:O    | 1:A:573:LEU:C   | 0.43     | 2.61        | 7      | 3     |
| 1:A:547:MET:O    | 1:A:549:ASN:N   | 0.43     | 2.52        | 4      | 1     |
| 2:C:55:THR:C     | 2:C:57:SER:N    | 0.43     | 2.77        | 7      | 1     |
| 1:A:574:TYR:O    | 1:A:575:MET:O   | 0.43     | 2.37        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:552:GLU:OE2  | 2:B:42:ARG:NE    | 0.43     | 2.52        | 10     | 1     |
| 1:A:558:LEU:H    | 1:A:558:LEU:HD23 | 0.42     | 1.73        | 3      | 1     |
| 1:A:494:GLY:C    | 1:A:496:ALA:H    | 0.42     | 2.20        | 6      | 1     |
| 1:A:557:GLU:C    | 1:A:558:LEU:HD22 | 0.42     | 2.38        | 9      | 1     |
| 2:B:4:PHE:O      | 2:B:67:LEU:HD12  | 0.42     | 2.14        | 9      | 1     |
| 2:C:45:PHE:O     | 2:C:48:LYS:N     | 0.42     | 2.51        | 9      | 1     |
| 1:A:526:ALA:O    | 1:A:527:SER:C    | 0.42     | 2.62        | 1      | 1     |
| 1:A:568:LEU:C    | 1:A:568:LEU:CD2  | 0.42     | 2.92        | 2      | 1     |
| 1:A:521:GLU:O    | 1:A:522:THR:C    | 0.42     | 2.61        | 9      | 2     |
| 2:B:60:ASN:N     | 2:B:60:ASN:ND2   | 0.42     | 2.67        | 2      | 1     |
| 2:C:42:ARG:CZ    | 2:C:49:GLN:NE2   | 0.42     | 2.82        | 2      | 1     |
| 1:A:581:VAL:O    | 1:A:582:ASP:C    | 0.42     | 2.61        | 10     | 1     |
| 1:A:510:LEU:N    | 1:A:511:PRO:HD2  | 0.42     | 2.30        | 7      | 5     |
| 1:A:601:VAL:O    | 1:A:605:SER:OG   | 0.42     | 2.37        | 3      | 1     |
| 1:A:517:ASP:CG   | 2:C:71:LEU:O     | 0.42     | 2.62        | 4      | 1     |
| 1:A:591:ILE:N    | 1:A:591:ILE:CD1  | 0.42     | 2.82        | 5      | 1     |
| 1:A:511:PRO:O    | 1:A:512:ILE:C    | 0.42     | 2.61        | 10     | 1     |
| 2:B:1:MET:O      | 2:B:17:VAL:N     | 0.42     | 2.52        | 2      | 1     |
| 2:C:58:ASP:C     | 2:C:59:TYR:CD1   | 0.42     | 2.98        | 8      | 1     |
| 2:C:38:PRO:O     | 2:C:39:ASP:C     | 0.42     | 2.62        | 6      | 2     |
| 1:A:511:PRO:C    | 1:A:513:ALA:H    | 0.42     | 2.23        | 10     | 2     |
| 1:A:515:SER:OG   | 1:A:517:ASP:CG   | 0.42     | 2.62        | 7      | 1     |
| 1:A:506:LEU:HD11 | 1:A:534:PHE:CE2  | 0.42     | 2.50        | 8      | 1     |
| 1:A:547:MET:O    | 1:A:548:ASP:C    | 0.42     | 2.62        | 10     | 1     |
| 2:B:1:MET:HB3    | 2:B:63:LYS:HB3   | 0.42     | 1.91        | 1      | 1     |
| 2:B:53:GLY:O     | 2:B:54:ARG:C     | 0.42     | 2.62        | 7      | 4     |
| 2:C:1:MET:HE2    | 2:C:19:PRO:CD    | 0.42     | 2.45        | 1      | 1     |
| 2:C:48:LYS:CD    | 2:C:48:LYS:N     | 0.42     | 2.83        | 1      | 1     |
| 1:A:560:THR:O    | 1:A:561:ASP:O    | 0.42     | 2.38        | 2      | 1     |
| 2:C:15:LEU:N     | 2:C:15:LEU:CD1   | 0.42     | 2.83        | 2      | 1     |
| 2:B:39:ASP:O     | 2:B:40:GLN:CG    | 0.42     | 2.68        | 2      | 2     |
| 2:B:1:MET:SD     | 2:B:17:VAL:CG2   | 0.42     | 3.08        | 3      | 1     |
| 1:A:494:GLY:C    | 1:A:496:ALA:N    | 0.42     | 2.77        | 6      | 1     |
| 1:A:526:ALA:C    | 1:A:528:LEU:N    | 0.42     | 2.77        | 8      | 1     |
| 2:C:58:ASP:OD1   | 2:C:58:ASP:N     | 0.41     | 2.53        | 2      | 1     |
| 1:A:515:SER:OG   | 1:A:517:ASP:OD2  | 0.41     | 2.38        | 7      | 1     |
| 2:B:73:LEU:C     | 2:B:73:LEU:HD12  | 0.41     | 2.40        | 8      | 1     |
| 1:A:501:LYS:C    | 1:A:502:ASN:OD1  | 0.41     | 2.62        | 9      | 1     |
| 2:B:9:THR:OG1    | 2:B:10:GLY:N     | 0.41     | 2.53        | 9      | 1     |
| 1:A:583:ASP:CG   | 2:B:6:LYS:NZ     | 0.41     | 2.78        | 10     | 1     |
| 1:A:502:ASN:CG   | 1:A:503:ASP:N    | 0.41     | 2.78        | 8      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:534:PHE:O    | 1:A:537:THR:O    | 0.41     | 2.38        | 7      | 1     |
| 1:A:541:ASP:N    | 2:B:74:ARG:NH2   | 0.41     | 2.68        | 9      | 1     |
| 1:A:553:ARG:O    | 1:A:554:THR:OG1  | 0.41     | 2.38        | 9      | 1     |
| 1:A:524:ALA:O    | 1:A:527:SER:OG   | 0.41     | 2.38        | 10     | 1     |
| 2:C:58:ASP:O     | 2:C:59:TYR:CG    | 0.41     | 2.73        | 5      | 1     |
| 1:A:505:VAL:O    | 1:A:509:LEU:HB2  | 0.41     | 2.15        | 10     | 1     |
| 1:A:599:ILE:O    | 1:A:602:LEU:N    | 0.41     | 2.53        | 1      | 1     |
| 1:A:507:GLY:C    | 1:A:508:LEU:HD12 | 0.41     | 2.41        | 8      | 1     |
| 1:A:512:ILE:O    | 1:A:512:ILE:HG22 | 0.41     | 2.14        | 1      | 1     |
| 1:A:561:ASP:O    | 1:A:561:ASP:OD1  | 0.41     | 2.38        | 1      | 1     |
| 1:A:515:SER:OG   | 1:A:518:LEU:HD11 | 0.41     | 2.14        | 4      | 1     |
| 1:A:532:HIS:ND1  | 1:A:532:HIS:N    | 0.41     | 2.69        | 4      | 1     |
| 1:A:585:LEU:HD12 | 1:A:585:LEU:N    | 0.41     | 2.31        | 4      | 1     |
| 1:A:512:ILE:HD11 | 2:C:9:THR:CG2    | 0.41     | 2.44        | 9      | 1     |
| 2:B:25:ASN:ND2   | 2:B:25:ASN:N     | 0.41     | 2.68        | 10     | 1     |
| 1:A:521:GLU:O    | 1:A:523:ALA:N    | 0.41     | 2.53        | 1      | 1     |
| 2:B:60:ASN:O     | 2:B:60:ASN:ND2   | 0.41     | 2.52        | 1      | 1     |
| 2:C:8:LEU:C      | 2:C:9:THR:CG2    | 0.41     | 2.94        | 2      | 1     |
| 1:A:587:THR:O    | 1:A:588:ILE:C    | 0.41     | 2.64        | 10     | 2     |
| 2:C:59:TYR:O     | 2:C:60:ASN:C     | 0.41     | 2.62        | 9      | 1     |
| 1:A:528:LEU:HD23 | 1:A:528:LEU:O    | 0.41     | 2.16        | 2      | 1     |
| 2:C:7:THR:OG1    | 2:C:10:GLY:C     | 0.41     | 2.64        | 4      | 1     |
| 2:C:32:ASP:O     | 2:C:32:ASP:OD1   | 0.41     | 2.38        | 5      | 1     |
| 1:A:558:LEU:N    | 1:A:558:LEU:CD2  | 0.41     | 2.83        | 7      | 1     |
| 2:C:8:LEU:CD1    | 2:C:70:VAL:HG13  | 0.41     | 2.46        | 8      | 1     |
| 1:A:498:ALA:O    | 1:A:499:GLY:C    | 0.41     | 2.61        | 10     | 1     |
| 1:A:541:ASP:C    | 1:A:544:THR:OG1  | 0.41     | 2.64        | 1      | 1     |
| 2:C:7:THR:CG2    | 2:C:11:LYS:O     | 0.41     | 2.63        | 7      | 1     |
| 1:A:541:ASP:N    | 2:B:74:ARG:HH21  | 0.41     | 2.13        | 9      | 1     |
| 1:A:492:GLY:O    | 1:A:493:LEU:C    | 0.41     | 2.64        | 10     | 1     |
| 1:A:568:LEU:HD23 | 1:A:568:LEU:O    | 0.40     | 2.16        | 2      | 1     |
| 1:A:523:ALA:O    | 1:A:524:ALA:C    | 0.40     | 2.64        | 8      | 1     |
| 2:C:18:GLU:O     | 2:C:21:ASP:N     | 0.40     | 2.49        | 3      | 1     |
| 1:A:560:THR:HG22 | 1:A:561:ASP:H    | 0.40     | 1.76        | 5      | 1     |
| 1:A:561:ASP:C    | 1:A:561:ASP:OD1  | 0.40     | 2.64        | 5      | 1     |
| 1:A:553:ARG:HG3  | 1:A:556:ILE:HD12 | 0.40     | 1.93        | 8      | 1     |
| 1:A:530:LEU:O    | 1:A:531:ALA:C    | 0.40     | 2.64        | 1      | 1     |
| 2:C:27:LYS:NZ    | 2:C:41:GLN:O     | 0.40     | 2.43        | 3      | 1     |
| 2:B:70:VAL:CG1   | 2:B:71:LEU:N     | 0.40     | 2.84        | 8      | 2     |
| 2:C:71:LEU:O     | 2:C:72:ARG:O     | 0.40     | 2.40        | 8      | 1     |
| 1:A:510:LEU:HD21 | 2:B:74:ARG:O     | 0.40     | 2.17        | 9      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 2:B:60:ASN:HD22 | 2:B:60:ASN:N    | 0.40     | 2.13        | 9      | 1     |
| 2:B:67:LEU:HD12 | 2:B:67:LEU:N    | 0.40     | 2.31        | 9      | 1     |
| 1:A:493:LEU:N   | 1:A:493:LEU:CD1 | 0.40     | 2.85        | 10     | 1     |
| 1:A:489:ALA:C   | 1:A:491:LEU:N   | 0.40     | 2.79        | 4      | 1     |
| 1:A:578:GLY:O   | 1:A:582:ASP:OD2 | 0.40     | 2.40        | 4      | 1     |
| 1:A:580:GLN:CD  | 1:A:580:GLN:H   | 0.40     | 2.23        | 4      | 1     |
| 2:C:32:ASP:OD1  | 2:C:32:ASP:C    | 0.40     | 2.64        | 5      | 1     |
| 1:A:598:ALA:O   | 1:A:599:ILE:C   | 0.40     | 2.63        | 8      | 1     |
| 2:C:46:ALA:O    | 2:C:47:GLY:C    | 0.40     | 2.64        | 8      | 1     |
| 1:A:560:THR:O   | 1:A:561:ASP:CG  | 0.40     | 2.65        | 10     | 1     |
| 1:A:560:THR:O   | 1:A:561:ASP:OD1 | 0.40     | 2.39        | 10     | 1     |
| 2:C:22:THR:O    | 2:C:25:ASN:N    | 0.40     | 2.55        | 10     | 1     |
| 1:A:509:LEU:O   | 1:A:510:LEU:C   | 0.40     | 2.63        | 1      | 1     |
| 1:A:529:ALA:O   | 1:A:530:LEU:C   | 0.40     | 2.65        | 2      | 1     |
| 1:A:596:THR:C   | 1:A:598:ALA:N   | 0.40     | 2.79        | 5      | 1     |
| 2:C:8:LEU:O     | 2:C:9:THR:CB    | 0.40     | 2.69        | 5      | 1     |
| 2:C:8:LEU:O     | 2:C:8:LEU:HD23  | 0.40     | 2.16        | 8      | 1     |
| 2:B:71:LEU:C    | 2:B:72:ARG:O    | 0.40     | 2.64        | 9      | 1     |
| 1:A:551:LEU:C   | 1:A:553:ARG:N   | 0.40     | 2.79        | 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     | 122/131 (93%)   | 74±5 (61±4%) | 34±5 (28±4%) | 14±4 (12±3%) | 1           | 7  |
| 2   | B     | 74/76 (97%)     | 57±2 (77±2%) | 11±2 (15±2%) | 6±1 (8±2%)   | 1           | 12 |
| 2   | C     | 71/76 (93%)     | 56±3 (79±4%) | 10±2 (15±3%) | 4±2 (6±2%)   | 2           | 18 |
| All | All   | 2670/2830 (94%) | 1869 (70%)   | 551 (21%)    | 250 (9%)     | 1           | 10 |

All 73 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     | 555 | ALA  | 10             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 592 | GLU  | 10             |
| 2   | B     | 35  | GLY  | 10             |
| 2   | B     | 39  | ASP  | 10             |
| 2   | B     | 54  | ARG  | 10             |
| 2   | C     | 35  | GLY  | 10             |
| 1   | A     | 562 | TRP  | 9              |
| 1   | A     | 519 | PRO  | 8              |
| 2   | C     | 54  | ARG  | 8              |
| 1   | A     | 557 | GLU  | 7              |
| 2   | B     | 46  | ALA  | 7              |
| 1   | A     | 554 | THR  | 7              |
| 2   | B     | 72  | ARG  | 7              |
| 1   | A     | 517 | ASP  | 6              |
| 2   | C     | 39  | ASP  | 6              |
| 2   | C     | 10  | GLY  | 6              |
| 1   | A     | 556 | ILE  | 6              |
| 1   | A     | 553 | ARG  | 5              |
| 1   | A     | 507 | GLY  | 5              |
| 1   | A     | 518 | LEU  | 4              |
| 1   | A     | 521 | GLU  | 4              |
| 1   | A     | 560 | THR  | 4              |
| 1   | A     | 561 | ASP  | 4              |
| 1   | A     | 607 | ALA  | 4              |
| 1   | A     | 594 | PRO  | 4              |
| 1   | A     | 500 | SER  | 4              |
| 1   | A     | 577 | GLN  | 4              |
| 1   | A     | 542 | ILE  | 3              |
| 1   | A     | 575 | MET  | 3              |
| 2   | B     | 73  | LEU  | 3              |
| 2   | C     | 8   | LEU  | 3              |
| 2   | C     | 9   | THR  | 3              |
| 2   | B     | 75  | GLY  | 3              |
| 2   | B     | 48  | LYS  | 2              |
| 2   | B     | 34  | GLU  | 2              |
| 1   | A     | 498 | ALA  | 2              |
| 1   | A     | 564 | ARG  | 2              |
| 1   | A     | 537 | THR  | 2              |
| 1   | A     | 544 | THR  | 2              |
| 1   | A     | 559 | LYS  | 2              |
| 1   | A     | 576 | GLY  | 2              |
| 1   | A     | 579 | GLU  | 2              |
| 1   | A     | 516 | THR  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 512 | ILE  | 2              |
| 2   | B     | 8   | LEU  | 2              |
| 2   | C     | 72  | ARG  | 2              |
| 2   | B     | 10  | GLY  | 1              |
| 2   | C     | 61  | ILE  | 1              |
| 1   | A     | 541 | ASP  | 1              |
| 2   | B     | 47  | GLY  | 1              |
| 1   | A     | 514 | ALA  | 1              |
| 1   | A     | 533 | VAL  | 1              |
| 1   | A     | 573 | LEU  | 1              |
| 2   | B     | 19  | PRO  | 1              |
| 2   | B     | 62  | GLN  | 1              |
| 2   | C     | 19  | PRO  | 1              |
| 2   | C     | 62  | GLN  | 1              |
| 1   | A     | 578 | GLY  | 1              |
| 1   | A     | 595 | MET  | 1              |
| 1   | A     | 596 | THR  | 1              |
| 2   | B     | 53  | GLY  | 1              |
| 2   | B     | 74  | ARG  | 1              |
| 1   | A     | 536 | GLY  | 1              |
| 2   | C     | 21  | ASP  | 1              |
| 2   | C     | 34  | GLU  | 1              |
| 2   | C     | 47  | GLY  | 1              |
| 1   | A     | 574 | TYR  | 1              |
| 1   | A     | 491 | LEU  | 1              |
| 1   | A     | 520 | ILE  | 1              |
| 1   | A     | 550 | PHE  | 1              |
| 2   | C     | 46  | ALA  | 1              |
| 1   | A     | 572 | ILE  | 1              |
| 1   | A     | 499 | 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     | 95/102 (93%) | 88±1 (93±1%) | 7±1 (7±1%) | 15 64       |
| 2   | B     | 68/68 (100%) | 64±1 (95±1%) | 4±1 (5±1%) | 21 71       |

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| Mol | Chain | Analysed        | Rotameric    | Outliers   | Percentiles |
|-----|-------|-----------------|--------------|------------|-------------|
| 2   | C     | 66/68 (97%)     | 61±1 (92±2%) | 5±1 (8±2%) | 14 62       |
| All | All   | 2290/2380 (96%) | 2136 (93%)   | 154 (7%)   | 17 65       |

All 45 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     | 546 | ILE  | 10             |
| 2   | B     | 52  | ASP  | 10             |
| 2   | C     | 52  | ASP  | 10             |
| 2   | B     | 20  | SER  | 8              |
| 2   | C     | 20  | SER  | 8              |
| 1   | A     | 556 | ILE  | 8              |
| 1   | A     | 554 | THR  | 7              |
| 2   | B     | 1   | MET  | 7              |
| 2   | C     | 70  | VAL  | 7              |
| 1   | A     | 516 | THR  | 6              |
| 1   | A     | 548 | ASP  | 5              |
| 2   | C     | 11  | LYS  | 4              |
| 1   | A     | 530 | LEU  | 4              |
| 1   | A     | 537 | THR  | 4              |
| 2   | C     | 13  | ILE  | 4              |
| 1   | A     | 518 | LEU  | 3              |
| 1   | A     | 593 | HIS  | 3              |
| 2   | B     | 8   | LEU  | 3              |
| 2   | C     | 25  | ASN  | 3              |
| 1   | A     | 515 | SER  | 3              |
| 2   | C     | 9   | THR  | 3              |
| 2   | B     | 25  | ASN  | 3              |
| 2   | C     | 8   | LEU  | 3              |
| 2   | C     | 1   | MET  | 2              |
| 1   | A     | 587 | THR  | 2              |
| 2   | B     | 60  | ASN  | 2              |
| 2   | C     | 58  | ASP  | 2              |
| 1   | A     | 553 | ARG  | 2              |
| 1   | A     | 522 | THR  | 2              |
| 1   | A     | 582 | ASP  | 1              |
| 1   | A     | 596 | THR  | 1              |
| 2   | B     | 13  | ILE  | 1              |
| 1   | A     | 493 | LEU  | 1              |
| 2   | B     | 18  | GLU  | 1              |
| 1   | A     | 560 | THR  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 2   | C     | 21  | ASP  | 1              |
| 2   | C     | 60  | ASN  | 1              |
| 2   | C     | 66  | THR  | 1              |
| 2   | C     | 18  | GLU  | 1              |
| 1   | A     | 517 | ASP  | 1              |
| 1   | A     | 497 | PHE  | 1              |
| 2   | B     | 48  | LYS  | 1              |
| 1   | A     | 509 | LEU  | 1              |
| 1   | A     | 545 | SER  | 1              |
| 2   | B     | 71  | LEU  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 28% for the well-defined parts and 27% 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                  | 1034 |
| Number of shifts mapped to atoms        | 1034 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 96       | $-0.46 \pm 0.14$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 92       | $0.23 \pm 0.10$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 0        | —                               | None (insufficient data)   |
| $^{15}\text{N}$        | 63       | $0.81 \pm 0.56$                 | None needed (imprecise)    |

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 28%, i.e. 1016 atoms were assigned a chemical shift out of a possible 3655. 0 out of 50 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 322/1352 (24%) | 164/551 (30%)  | 95/540 (18%)    | 63/261 (24%)    |
| Sidechain | 674/2156 (31%) | 470/1413 (33%) | 204/679 (30%)   | 0/64 (0%)       |

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|          | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|-----------------|----------------|-----------------|-----------------|
| Aromatic | 20/147 (14%)    | 20/74 (27%)    | 0/68 (0%)       | 0/5 (0%)        |
| Overall  | 1016/3655 (28%) | 654/2038 (32%) | 299/1287 (23%)  | 63/330 (19%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 1034 atoms were assigned a chemical shift out of a possible 3815. 0 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 324/1421 (23%)  | 165/581 (28%)  | 96/566 (17%)    | 63/274 (23%)    |
| Sidechain | 686/2238 (31%)  | 478/1466 (33%) | 208/704 (30%)   | 0/68 (0%)       |
| Aromatic  | 24/156 (15%)    | 24/78 (31%)    | 0/73 (0%)       | 0/5 (0%)        |
| Overall   | 1034/3815 (27%) | 667/2125 (31%) | 304/1343 (23%)  | 63/347 (18%)    |

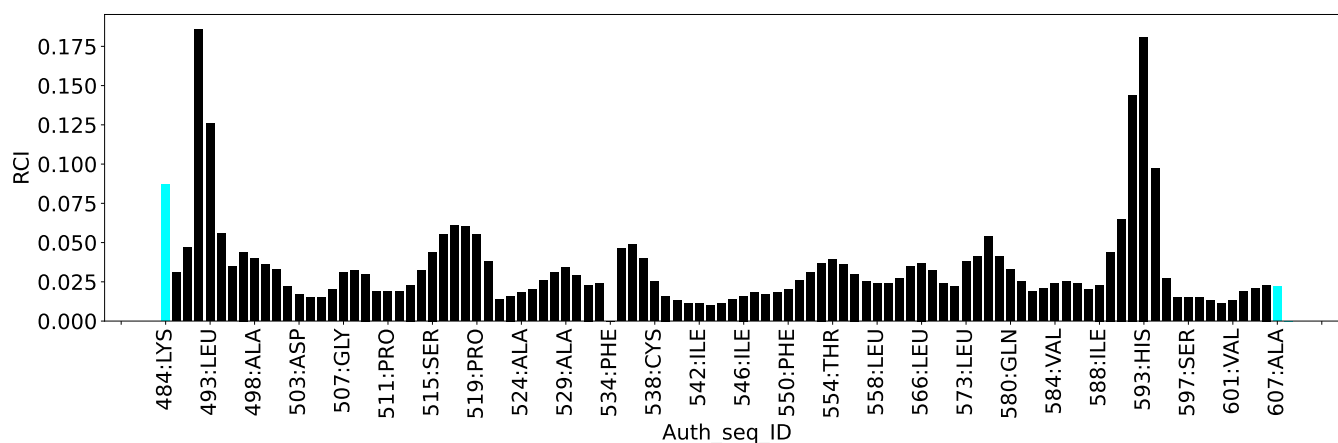
#### 7.1.4 Statistically unusual chemical shifts [i](#)

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                                | 6379  |
| Intra-residue ( $ i-j =0$ )                              | 1692  |
| Sequential ( $ i-j =1$ )                                 | 980   |
| Medium range ( $ i-j >1$ and $ i-j <5$ )                 | 1029  |
| Long range ( $ i-j \geq 5$ )                             | 2381  |
| Inter-chain                                              | 117   |
| Hydrogen bond restraints                                 | 180   |
| Disulfide bond restraints                                | 0     |
| Total dihedral-angle restraints                          | 249   |
| Number of unmapped restraints                            | 0     |
| Number of restraints per residue                         | 23.4  |
| Number of long range restraints per residue <sup>1</sup> | 8.5   |

<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)  | 17.7                                   | 0.2     |
| 0.2-0.5 (Medium) | 32.5                                   | 0.5     |
| >0.5 (Large)     | 33.9                                   | 2.97    |

### 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)   | 3.7                                    | 7.73    |
| 10.0-20.0 (Medium) | None                                   | None    |
| >20.0 (Large)      | 0.4                                    | 55.81   |

## 9 Distance violation analysis

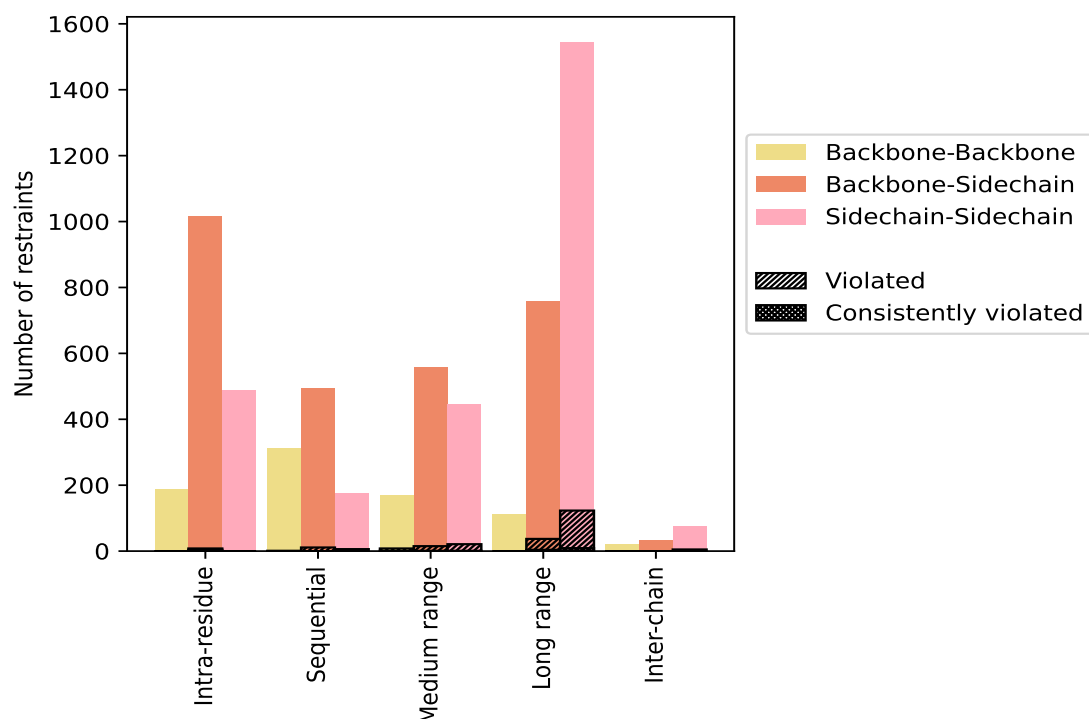
### 9.1 Summary of distance violations

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

| Restrains type                                                              | Count       | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|-----------------------------------------------------------------------------|-------------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|                                                                             |             |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| <b>Intra-residue (<math> i-j =0</math>)</b>                                 | <b>1692</b> | <b>26.5</b>    | <b>8</b>              | <b>0.5</b>     | <b>0.1</b>     | <b>4</b>                           | <b>0.2</b>     | <b>0.1</b>     |
| Backbone-Backbone                                                           | 188         | 2.9            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 1016        | 15.9           | 8                     | 0.8            | 0.1            | 4                                  | 0.4            | 0.1            |
| Sidechain-Sidechain                                                         | 488         | 7.7            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Sequential (<math> i-j =1</math>)</b>                                    | <b>980</b>  | <b>15.4</b>    | <b>18</b>             | <b>1.8</b>     | <b>0.3</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 311         | 4.9            | 1                     | 0.3            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 495         | 7.8            | 11                    | 2.2            | 0.2            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 174         | 2.7            | 6                     | 3.4            | 0.1            | 0                                  | 0.0            | 0.0            |
| <b>Medium range (<math> i-j &gt;1</math> &amp; <math> i-j &lt;5</math>)</b> | <b>1029</b> | <b>16.1</b>    | <b>42</b>             | <b>4.1</b>     | <b>0.7</b>     | <b>3</b>                           | <b>0.3</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 168         | 2.6            | 8                     | 4.8            | 0.1            | 1                                  | 0.6            | 0.0            |
| Backbone-Sidechain                                                          | 416         | 6.5            | 13                    | 3.1            | 0.2            | 1                                  | 0.2            | 0.0            |
| Sidechain-Sidechain                                                         | 445         | 7.0            | 21                    | 4.7            | 0.3            | 1                                  | 0.2            | 0.0            |
| <b>Long range (<math> i-j \geq 5</math>)</b>                                | <b>2381</b> | <b>37.3</b>    | <b>160</b>            | <b>6.7</b>     | <b>2.5</b>     | <b>13</b>                          | <b>0.5</b>     | <b>0.2</b>     |
| Backbone-Backbone                                                           | 112         | 1.8            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 725         | 11.4           | 37                    | 5.1            | 0.6            | 4                                  | 0.6            | 0.1            |
| Sidechain-Sidechain                                                         | 1544        | 24.2           | 123                   | 8.0            | 1.9            | 9                                  | 0.6            | 0.1            |
| <b>Inter-chain</b>                                                          | <b>117</b>  | <b>1.8</b>     | <b>2</b>              | <b>1.7</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| Backbone-Backbone                                                           | 19          | 0.3            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Backbone-Sidechain                                                          | 31          | 0.5            | 0                     | 0.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| Sidechain-Sidechain                                                         | 67          | 1.1            | 2                     | 3.0            | 0.0            | 0                                  | 0.0            | 0.0            |
| <b>Hydrogen bond</b>                                                        | <b>180</b>  | <b>2.8</b>     | <b>5</b>              | <b>2.8</b>     | <b>0.1</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Disulfide bond</b>                                                       | <b>0</b>    | <b>0.0</b>     | <b>0</b>              | <b>0.0</b>     | <b>0.0</b>     | <b>0</b>                           | <b>0.0</b>     | <b>0.0</b>     |
| <b>Total</b>                                                                | <b>6379</b> | <b>100.0</b>   | <b>235</b>            | <b>3.7</b>     | <b>3.7</b>     | <b>20</b>                          | <b>0.3</b>     | <b>0.3</b>     |
| Backbone-Backbone                                                           | 798         | 12.5           | 9                     | 1.1            | 0.1            | 1                                  | 0.1            | 0.0            |
| Backbone-Sidechain                                                          | 2855        | 44.8           | 71                    | 2.5            | 1.1            | 9                                  | 0.3            | 0.1            |
| Sidechain-Sidechain                                                         | 2726        | 42.7           | 155                   | 5.7            | 2.4            | 10                                 | 0.4            | 0.2            |

<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 disulfide bonds are counted in their appropriate category on the x-axis

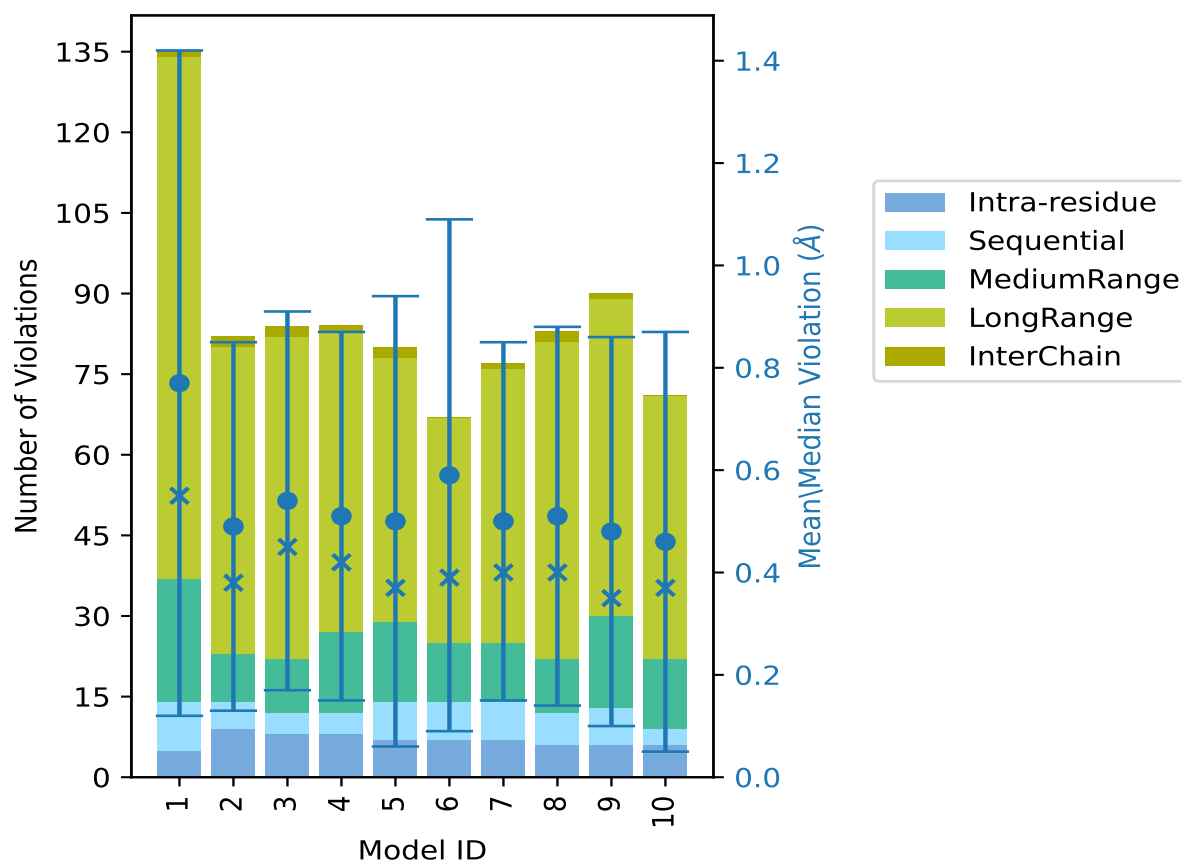
## 9.2 Distance violation statistics for each model [i](#)

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        | 5                    | 9               | 23              | 97              | 1               | 135   | 0.77     | 2.97    | 0.65                | 0.55       |
| 2        | 9                    | 5               | 9               | 57              | 2               | 82    | 0.49     | 1.89    | 0.36                | 0.38       |
| 3        | 8                    | 4               | 10              | 60              | 2               | 84    | 0.54     | 2.22    | 0.37                | 0.45       |
| 4        | 8                    | 4               | 15              | 56              | 1               | 84    | 0.51     | 1.6     | 0.36                | 0.42       |
| 5        | 7                    | 7               | 15              | 49              | 2               | 80    | 0.5      | 1.9     | 0.44                | 0.37       |
| 6        | 7                    | 7               | 11              | 42              | 0               | 67    | 0.59     | 2.19    | 0.5                 | 0.39       |
| 7        | 7                    | 7               | 11              | 51              | 1               | 77    | 0.5      | 1.78    | 0.35                | 0.4        |
| 8        | 6                    | 6               | 10              | 59              | 2               | 83    | 0.51     | 2.02    | 0.37                | 0.4        |
| 9        | 6                    | 7               | 17              | 59              | 1               | 90    | 0.48     | 1.78    | 0.38                | 0.35       |
| 10       | 6                    | 3               | 13              | 49              | 0               | 71    | 0.46     | 2.42    | 0.41                | 0.37       |

<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, 5969(IR:1684, SQ:962, MR:987, LR:2221, IC:115) 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>       | %    |
| 2                             | 8               | 23              | 66              | 1               | 100   | 1                        | 10.0 |
| 0                             | 2               | 3               | 15              | 0               | 20    | 2                        | 20.0 |
| 1                             | 3               | 3               | 18              | 1               | 26    | 3                        | 30.0 |

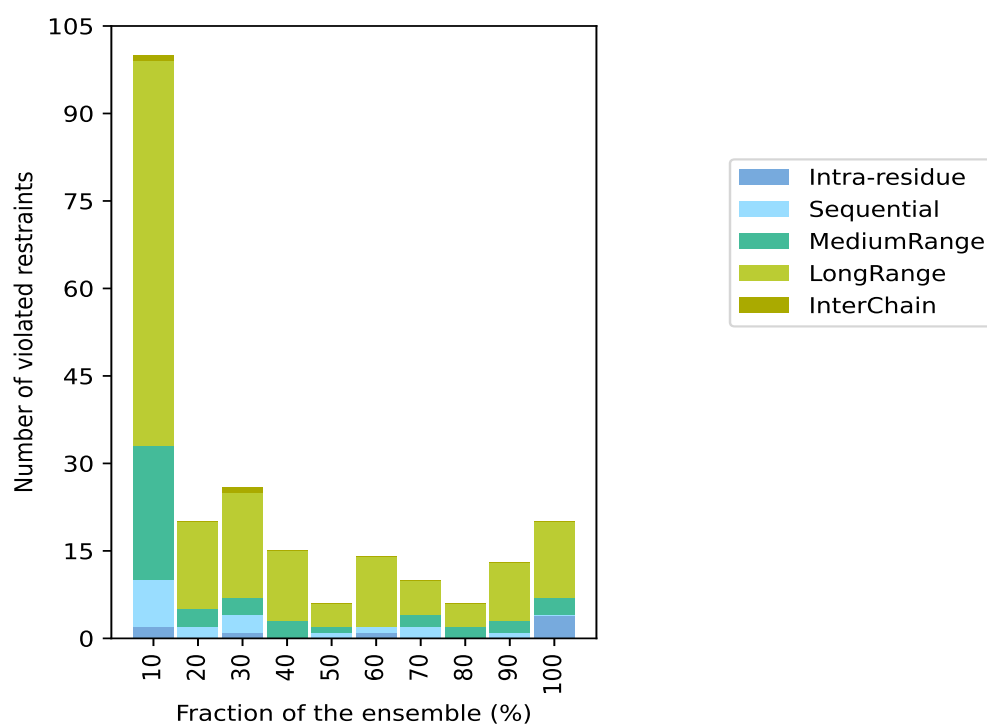
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| Number of violated restraints |                 |                 |                 |                 |       | Fraction of the ensemble |       |
|-------------------------------|-----------------|-----------------|-----------------|-----------------|-------|--------------------------|-------|
| 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               | 3               | 12              | 0               | 15    | 4                        | 40.0  |
| 0                             | 1               | 1               | 4               | 0               | 6     | 5                        | 50.0  |
| 1                             | 1               | 0               | 12              | 0               | 14    | 6                        | 60.0  |
| 0                             | 2               | 2               | 6               | 0               | 10    | 7                        | 70.0  |
| 0                             | 0               | 2               | 4               | 0               | 6     | 8                        | 80.0  |
| 0                             | 1               | 2               | 10              | 0               | 13    | 9                        | 90.0  |
| 4                             | 0               | 3               | 13              | 0               | 20    | 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](#)

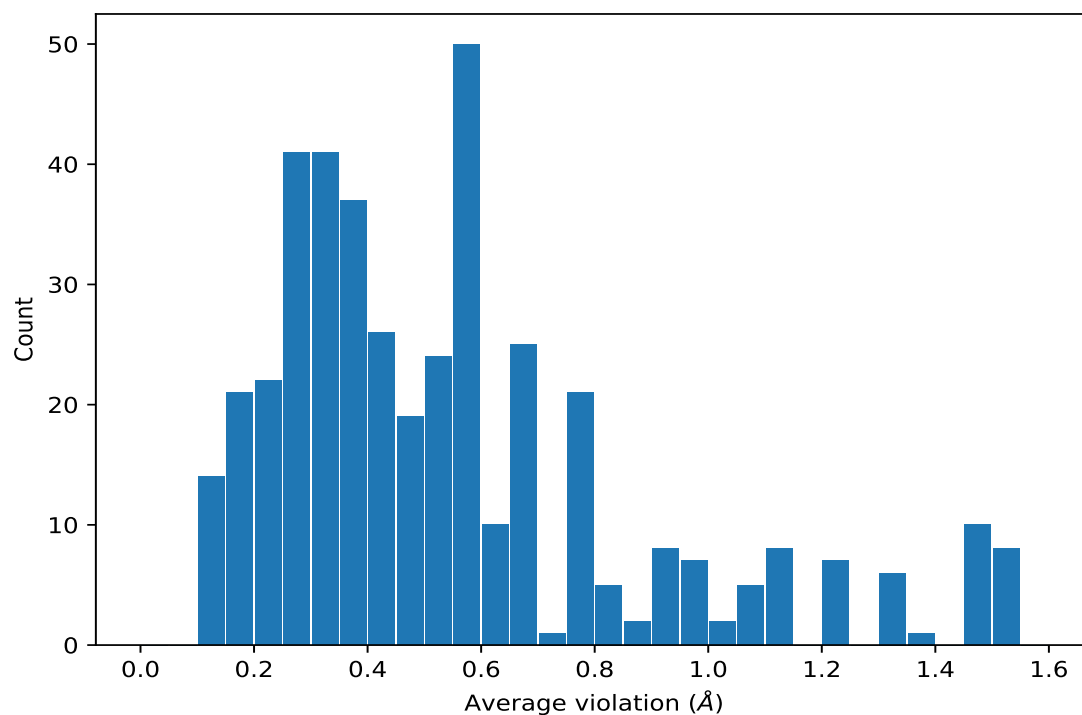


## 9.4 Most violated distance restraints in the ensemble [i](#)

### 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) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1450) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG11 | 10                  | 1.52     | 0.49                | 1.36       |
| (1,1450) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG12 | 10                  | 1.52     | 0.49                | 1.36       |
| (1,1450) | 2:1:B:MET:HE3    | 2:17:B:VAL:HG11 | 10                  | 1.52     | 0.49                | 1.36       |
| (1,1450) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG13 | 10                  | 1.52     | 0.49                | 1.36       |
| (1,1450) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG13 | 10                  | 1.52     | 0.49                | 1.36       |
| (1,1450) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG11 | 10                  | 1.52     | 0.49                | 1.36       |
| (1,3716) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG12 | 10                  | 1.47     | 0.32                | 1.36       |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12 | 10                  | 1.47     | 0.32                | 1.36       |
| (1,3716) | 2:1:C:MET:HE2    | 2:17:C:VAL:HG12 | 10                  | 1.47     | 0.32                | 1.36       |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG11 | 10                  | 1.47     | 0.32                | 1.36       |
| (1,3716) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG13 | 10                  | 1.47     | 0.32                | 1.36       |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 10                  | 1.31     | 0.35                | 1.28       |
| (1,1390) | 1:599:A:ILE:HD11 | 1:562:A:TRP:HZ3 | 10                  | 1.23     | 0.51                | 1.4        |
| (1,1390) | 1:599:A:ILE:HD13 | 1:562:A:TRP:HZ3 | 10                  | 1.23     | 0.51                | 1.4        |
| (1,1390) | 1:599:A:ILE:HD13 | 1:562:A:TRP:HZ2 | 10                  | 1.23     | 0.51                | 1.4        |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1390) | 1:599:A:ILE:HD11 | 1:562:A:TRP:HZ2 | 10                  | 1.23     | 0.51                | 1.4        |
| (1,1390) | 1:599:A:ILE:HD12 | 1:562:A:TRP:HZ3 | 10                  | 1.23     | 0.51                | 1.4        |
| (1,1390) | 1:599:A:ILE:HD12 | 1:562:A:TRP:HZ2 | 10                  | 1.23     | 0.51                | 1.4        |
| (1,1390) | 1:599:A:ILE:HD13 | 1:562:A:TRP:HD1 | 10                  | 1.23     | 0.51                | 1.4        |
| (1,1449) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG11 | 10                  | 1.14     | 0.49                | 0.98       |
| (1,1449) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG12 | 10                  | 1.14     | 0.49                | 0.98       |
| (1,1449) | 2:1:B:MET:HE3    | 2:17:B:VAL:HG11 | 10                  | 1.14     | 0.49                | 0.98       |
| (1,1449) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG13 | 10                  | 1.14     | 0.49                | 0.98       |
| (1,1449) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG13 | 10                  | 1.14     | 0.49                | 0.98       |
| (1,1449) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG11 | 10                  | 1.14     | 0.49                | 0.98       |
| (1,3715) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG12 | 10                  | 1.09     | 0.32                | 0.98       |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12 | 10                  | 1.09     | 0.32                | 0.98       |
| (1,3715) | 2:1:C:MET:HE2    | 2:17:C:VAL:HG12 | 10                  | 1.09     | 0.32                | 0.98       |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG11 | 10                  | 1.09     | 0.32                | 0.98       |
| (1,3715) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG13 | 10                  | 1.09     | 0.32                | 0.98       |
| (1,3634) | 2:66:B:THR:HG23  | 2:68:B:HIS:HB3  | 10                  | 0.98     | 0.16                | 1.02       |
| (1,3634) | 2:70:B:VAL:HG12  | 2:68:B:HIS:HB3  | 10                  | 0.98     | 0.16                | 1.02       |
| (1,3634) | 2:66:B:THR:HG21  | 2:68:B:HIS:HB3  | 10                  | 0.98     | 0.16                | 1.02       |
| (1,3634) | 2:66:B:THR:HG22  | 2:68:B:HIS:HB3  | 10                  | 0.98     | 0.16                | 1.02       |
| (1,3634) | 2:70:B:VAL:HG13  | 2:68:B:HIS:HB3  | 10                  | 0.98     | 0.16                | 1.02       |
| (1,1512) | 2:1:B:MET:HE2    | 2:67:B:LEU:HD21 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,1512) | 2:1:B:MET:HE1    | 2:67:B:LEU:HD12 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,1512) | 2:1:B:MET:HE3    | 2:67:B:LEU:HD11 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,1512) | 2:1:B:MET:HE1    | 2:67:B:LEU:HD11 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,1512) | 2:1:B:MET:HE2    | 2:67:B:LEU:HD13 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,1512) | 2:1:B:MET:HE3    | 2:67:B:LEU:HD13 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,1512) | 2:1:B:MET:HE1    | 2:67:B:LEU:HD13 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,1512) | 2:1:B:MET:HE2    | 2:67:B:LEU:HD11 | 10                  | 0.95     | 0.68                | 0.78       |
| (1,3778) | 2:1:C:MET:HE1    | 2:67:C:LEU:HD13 | 10                  | 0.77     | 0.75                | 0.46       |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD12 | 10                  | 0.77     | 0.75                | 0.46       |
| (1,3778) | 2:1:C:MET:HE3    | 2:67:C:LEU:HD12 | 10                  | 0.77     | 0.75                | 0.46       |
| (1,3778) | 2:1:C:MET:HE1    | 2:67:C:LEU:HD11 | 10                  | 0.77     | 0.75                | 0.46       |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD11 | 10                  | 0.77     | 0.75                | 0.46       |
| (1,3778) | 2:1:C:MET:HE3    | 2:67:C:LEU:HD11 | 10                  | 0.77     | 0.75                | 0.46       |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD13 | 10                  | 0.77     | 0.75                | 0.46       |
| (1,5311) | 2:41:C:GLN:H     | 2:71:C:LEU:HD22 | 10                  | 0.67     | 0.21                | 0.74       |
| (1,5311) | 2:41:C:GLN:H     | 2:69:C:LEU:HD13 | 10                  | 0.67     | 0.21                | 0.74       |
| (1,5311) | 2:41:C:GLN:H     | 2:69:C:LEU:HD11 | 10                  | 0.67     | 0.21                | 0.74       |
| (1,5311) | 2:41:C:GLN:H     | 2:71:C:LEU:HD21 | 10                  | 0.67     | 0.21                | 0.74       |
| (1,5311) | 2:41:C:GLN:H     | 2:69:C:LEU:HD12 | 10                  | 0.67     | 0.21                | 0.74       |
| (1,3833) | 2:3:C:ILE:HD13   | 2:3:C:ILE:HA    | 10                  | 0.64     | 0.03                | 0.64       |
| (1,3833) | 2:3:C:ILE:HD12   | 2:3:C:ILE:HA    | 10                  | 0.64     | 0.03                | 0.64       |

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| Key      | Atom-1         | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3833) | 2:3:C:ILE:HD11 | 2:3:C:ILE:HA    | 10                  | 0.64     | 0.03                | 0.64       |
| (1,1567) | 2:3:B:ILE:HD11 | 2:3:B:ILE:HA    | 10                  | 0.62     | 0.03                | 0.64       |
| (1,1567) | 2:3:B:ILE:HD13 | 2:3:B:ILE:HA    | 10                  | 0.62     | 0.03                | 0.64       |
| (1,1567) | 2:3:B:ILE:HD12 | 2:3:B:ILE:HA    | 10                  | 0.62     | 0.03                | 0.64       |
| (1,3759) | 2:1:C:MET:HE1  | 2:56:C:LEU:HD12 | 10                  | 0.57     | 0.29                | 0.47       |
| (1,3759) | 2:1:C:MET:HE3  | 2:56:C:LEU:HD13 | 10                  | 0.57     | 0.29                | 0.47       |
| (1,3759) | 2:1:C:MET:HE2  | 2:56:C:LEU:HD12 | 10                  | 0.57     | 0.29                | 0.47       |
| (1,3759) | 2:1:C:MET:HE3  | 2:56:C:LEU:HD11 | 10                  | 0.57     | 0.29                | 0.47       |
| (1,3759) | 2:1:C:MET:HE1  | 2:56:C:LEU:HD11 | 10                  | 0.57     | 0.29                | 0.47       |
| (1,3759) | 2:1:C:MET:HE3  | 2:56:C:LEU:HD12 | 10                  | 0.57     | 0.29                | 0.47       |
| (1,3759) | 2:1:C:MET:HE1  | 2:56:C:LEU:HD13 | 10                  | 0.57     | 0.29                | 0.47       |
| (1,3801) | 2:68:C:HIS:HA  | 2:5:C:VAL:HG12  | 10                  | 0.47     | 0.1                 | 0.44       |
| (1,3801) | 2:68:C:HIS:HA  | 2:5:C:VAL:HG11  | 10                  | 0.47     | 0.1                 | 0.44       |
| (1,3801) | 2:68:C:HIS:HA  | 2:5:C:VAL:HG13  | 10                  | 0.47     | 0.1                 | 0.44       |
| (1,4040) | 2:5:C:VAL:HA   | 2:66:C:THR:HG21 | 10                  | 0.4      | 0.08                | 0.42       |
| (1,4040) | 2:5:C:VAL:HA   | 2:66:C:THR:HG22 | 10                  | 0.4      | 0.08                | 0.42       |
| (1,4040) | 2:5:C:VAL:HA   | 2:66:C:THR:HG23 | 10                  | 0.4      | 0.08                | 0.42       |
| (1,4041) | 2:5:C:VAL:HA   | 2:66:C:THR:HG21 | 10                  | 0.4      | 0.08                | 0.4        |
| (1,4041) | 2:5:C:VAL:HA   | 2:66:C:THR:HG22 | 10                  | 0.4      | 0.08                | 0.4        |
| (1,4041) | 2:5:C:VAL:HA   | 2:66:C:THR:HG23 | 10                  | 0.4      | 0.08                | 0.4        |
| (1,3758) | 2:1:C:MET:HE1  | 2:56:C:LEU:HD12 | 10                  | 0.4      | 0.29                | 0.3        |
| (1,3758) | 2:1:C:MET:HE3  | 2:56:C:LEU:HD13 | 10                  | 0.4      | 0.29                | 0.3        |
| (1,3758) | 2:1:C:MET:HE2  | 2:56:C:LEU:HD12 | 10                  | 0.4      | 0.29                | 0.3        |
| (1,3758) | 2:1:C:MET:HE3  | 2:56:C:LEU:HD11 | 10                  | 0.4      | 0.29                | 0.3        |
| (1,3758) | 2:1:C:MET:HE1  | 2:56:C:LEU:HD11 | 10                  | 0.4      | 0.29                | 0.3        |
| (1,3758) | 2:1:C:MET:HE3  | 2:56:C:LEU:HD12 | 10                  | 0.4      | 0.29                | 0.3        |
| (1,3758) | 2:1:C:MET:HE1  | 2:56:C:LEU:HD13 | 10                  | 0.4      | 0.29                | 0.3        |
| (1,1588) | 2:29:B:LYS:HA  | 2:15:B:LEU:HD21 | 10                  | 0.39     | 0.23                | 0.36       |
| (1,1588) | 2:29:B:LYS:HA  | 2:15:B:LEU:HD13 | 10                  | 0.39     | 0.23                | 0.36       |
| (1,1588) | 2:29:B:LYS:HA  | 2:15:B:LEU:HD22 | 10                  | 0.39     | 0.23                | 0.36       |
| (1,1588) | 2:29:B:LYS:HA  | 2:15:B:LEU:HD11 | 10                  | 0.39     | 0.23                | 0.36       |
| (1,1588) | 2:29:B:LYS:HA  | 2:15:B:LEU:HD12 | 10                  | 0.39     | 0.23                | 0.36       |
| (1,3826) | 2:3:C:ILE:HA   | 2:3:C:ILE:HD13  | 10                  | 0.36     | 0.03                | 0.37       |
| (1,3826) | 2:3:C:ILE:HA   | 2:3:C:ILE:HD12  | 10                  | 0.36     | 0.03                | 0.37       |
| (1,3826) | 2:3:C:ILE:HA   | 2:3:C:ILE:HD11  | 10                  | 0.36     | 0.03                | 0.37       |
| (1,1560) | 2:3:B:ILE:HA   | 2:3:B:ILE:HD11  | 10                  | 0.34     | 0.03                | 0.36       |
| (1,1560) | 2:3:B:ILE:HA   | 2:3:B:ILE:HD13  | 10                  | 0.34     | 0.03                | 0.36       |
| (1,1560) | 2:3:B:ILE:HA   | 2:3:B:ILE:HD12  | 10                  | 0.34     | 0.03                | 0.36       |
| (1,5286) | 2:40:C:GLN:HG3 | 2:71:C:LEU:HD22 | 9                   | 1.49     | 0.43                | 1.43       |
| (1,5286) | 2:40:C:GLN:HG2 | 2:71:C:LEU:HD22 | 9                   | 1.49     | 0.43                | 1.43       |
| (1,5286) | 2:40:C:GLN:HG3 | 2:71:C:LEU:HD23 | 9                   | 1.49     | 0.43                | 1.43       |
| (1,5286) | 2:40:C:GLN:HG2 | 2:71:C:LEU:HD23 | 9                   | 1.49     | 0.43                | 1.43       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5286) | 2:40:C:GLN:HG2  | 2:71:C:LEU:HD21 | 9                   | 1.49     | 0.43                | 1.43       |
| (1,3020) | 2:40:B:GLN:HG3  | 2:71:B:LEU:HD23 | 9                   | 1.32     | 0.63                | 1.34       |
| (1,3020) | 2:40:B:GLN:HG2  | 2:71:B:LEU:HD23 | 9                   | 1.32     | 0.63                | 1.34       |
| (1,3020) | 2:40:B:GLN:HG2  | 2:71:B:LEU:HD21 | 9                   | 1.32     | 0.63                | 1.34       |
| (1,3020) | 2:40:B:GLN:HG3  | 2:71:B:LEU:HD22 | 9                   | 1.32     | 0.63                | 1.34       |
| (1,3020) | 2:40:B:GLN:HG3  | 2:71:B:LEU:HD11 | 9                   | 1.32     | 0.63                | 1.34       |
| (1,1841) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 9                   | 0.84     | 0.18                | 0.86       |
| (1,1841) | 2:6:B:LYS:HG2   | 2:66:B:THR:HG23 | 9                   | 0.84     | 0.18                | 0.86       |
| (1,1841) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG23 | 9                   | 0.84     | 0.18                | 0.86       |
| (1,1841) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG21 | 9                   | 0.84     | 0.18                | 0.86       |
| (1,5281) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD22 | 9                   | 0.65     | 0.26                | 0.59       |
| (1,5281) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD23 | 9                   | 0.65     | 0.26                | 0.59       |
| (1,5281) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD21 | 9                   | 0.65     | 0.26                | 0.59       |
| (3,259)  | 2:66:C:THR:HG21 | 2:67:C:LEU:HD23 | 9                   | 0.65     | 0.19                | 0.66       |
| (3,259)  | 2:66:C:THR:HG22 | 2:67:C:LEU:HD21 | 9                   | 0.65     | 0.19                | 0.66       |
| (3,259)  | 2:66:C:THR:HG21 | 2:67:C:LEU:HD21 | 9                   | 0.65     | 0.19                | 0.66       |
| (3,259)  | 2:66:C:THR:HG21 | 2:67:C:LEU:HD22 | 9                   | 0.65     | 0.19                | 0.66       |
| (3,259)  | 2:66:C:THR:HG23 | 2:67:C:LEU:HD21 | 9                   | 0.65     | 0.19                | 0.66       |
| (3,259)  | 2:66:C:THR:HG23 | 2:67:C:LEU:HD12 | 9                   | 0.65     | 0.19                | 0.66       |
| (2,4)    | 1:484:A:LYS:O   | 1:488:A:ALA:N   | 9                   | 0.62     | 0.23                | 0.68       |
| (1,1493) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD12 | 9                   | 0.57     | 0.44                | 0.38       |
| (1,1493) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD13 | 9                   | 0.57     | 0.44                | 0.38       |
| (1,1493) | 2:1:B:MET:HE1   | 2:56:B:LEU:HD11 | 9                   | 0.57     | 0.44                | 0.38       |
| (1,1493) | 2:1:B:MET:HE3   | 2:56:B:LEU:HD13 | 9                   | 0.57     | 0.44                | 0.38       |
| (1,1493) | 2:1:B:MET:HE1   | 2:56:B:LEU:HD13 | 9                   | 0.57     | 0.44                | 0.38       |
| (1,1493) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD11 | 9                   | 0.57     | 0.44                | 0.38       |
| (1,5280) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD22 | 9                   | 0.56     | 0.26                | 0.5        |
| (1,5280) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD23 | 9                   | 0.56     | 0.26                | 0.5        |
| (1,5280) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD21 | 9                   | 0.56     | 0.26                | 0.5        |
| (1,1839) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 9                   | 0.53     | 0.18                | 0.55       |
| (1,1839) | 2:6:B:LYS:HG2   | 2:66:B:THR:HG23 | 9                   | 0.53     | 0.18                | 0.55       |
| (1,1839) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG23 | 9                   | 0.53     | 0.18                | 0.55       |
| (1,1839) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG21 | 9                   | 0.53     | 0.18                | 0.55       |
| (2,3)    | 1:484:A:LYS:O   | 1:488:A:ALA:H   | 9                   | 0.52     | 0.24                | 0.55       |
| (1,1452) | 2:1:B:MET:HE2   | 2:17:B:VAL:HG21 | 9                   | 0.38     | 0.44                | 0.22       |
| (1,1452) | 2:1:B:MET:HE2   | 2:17:B:VAL:HG22 | 9                   | 0.38     | 0.44                | 0.22       |
| (1,1452) | 2:1:B:MET:HE3   | 2:17:B:VAL:HG22 | 9                   | 0.38     | 0.44                | 0.22       |
| (1,1452) | 2:1:B:MET:HE1   | 2:17:B:VAL:HG21 | 9                   | 0.38     | 0.44                | 0.22       |
| (1,1452) | 2:1:B:MET:HE2   | 2:17:B:VAL:HG23 | 9                   | 0.38     | 0.44                | 0.22       |
| (1,5302) | 2:41:C:GLN:HA   | 2:71:C:LEU:HD21 | 9                   | 0.37     | 0.12                | 0.32       |
| (1,5302) | 2:41:C:GLN:HA   | 2:71:C:LEU:HD22 | 9                   | 0.37     | 0.12                | 0.32       |
| (1,5302) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD13 | 9                   | 0.37     | 0.12                | 0.32       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,5302) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD11 | 9                   | 0.37     | 0.12                | 0.32       |
| (1,5302) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD12 | 9                   | 0.37     | 0.12                | 0.32       |
| (1,5301) | 2:41:C:GLN:HA   | 2:71:C:LEU:HD21 | 9                   | 0.33     | 0.12                | 0.28       |
| (1,5301) | 2:41:C:GLN:HA   | 2:71:C:LEU:HD22 | 9                   | 0.33     | 0.12                | 0.28       |
| (1,5301) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD13 | 9                   | 0.33     | 0.12                | 0.28       |
| (1,5301) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD11 | 9                   | 0.33     | 0.12                | 0.28       |
| (1,5301) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD12 | 9                   | 0.33     | 0.12                | 0.28       |
| (1,4206) | 2:14:C:THR:HG21 | 2:14:C:THR:H    | 9                   | 0.16     | 0.04                | 0.17       |
| (1,4206) | 2:14:C:THR:HG23 | 2:14:C:THR:H    | 9                   | 0.16     | 0.04                | 0.17       |
| (1,1940) | 2:14:B:THR:HG23 | 2:14:B:THR:H    | 9                   | 0.14     | 0.02                | 0.14       |
| (1,1940) | 2:14:B:THR:HG22 | 2:14:B:THR:H    | 9                   | 0.14     | 0.02                | 0.14       |
| (1,1940) | 2:14:B:THR:HG21 | 2:14:B:THR:H    | 9                   | 0.14     | 0.02                | 0.14       |
| (1,256)  | 1:515:A:SER:HA  | 1:518:A:LEU:H   | 8                   | 1.39     | 0.58                | 1.24       |
| (1,3045) | 2:41:B:GLN:H    | 2:69:B:LEU:HD13 | 8                   | 0.58     | 0.24                | 0.61       |
| (1,3045) | 2:41:B:GLN:H    | 2:69:B:LEU:HD23 | 8                   | 0.58     | 0.24                | 0.61       |
| (1,3045) | 2:41:B:GLN:H    | 2:69:B:LEU:HD12 | 8                   | 0.58     | 0.24                | 0.61       |
| (1,3045) | 2:41:B:GLN:H    | 2:71:B:LEU:HD21 | 8                   | 0.58     | 0.24                | 0.61       |
| (1,3045) | 2:41:B:GLN:H    | 2:69:B:LEU:HD11 | 8                   | 0.58     | 0.24                | 0.61       |
| (1,3045) | 2:41:B:GLN:H    | 2:71:B:LEU:HD23 | 8                   | 0.58     | 0.24                | 0.61       |
| (1,3699) | 2:1:C:MET:HE1   | 2:3:C:ILE:HD13  | 8                   | 0.53     | 0.58                | 0.34       |
| (1,3699) | 2:1:C:MET:HE2   | 2:3:C:ILE:HD12  | 8                   | 0.53     | 0.58                | 0.34       |
| (1,3699) | 2:1:C:MET:HE1   | 2:3:C:ILE:HD12  | 8                   | 0.53     | 0.58                | 0.34       |
| (1,3699) | 2:1:C:MET:HE2   | 2:3:C:ILE:HD11  | 8                   | 0.53     | 0.58                | 0.34       |
| (1,3699) | 2:1:C:MET:HE3   | 2:3:C:ILE:HD11  | 8                   | 0.53     | 0.58                | 0.34       |
| (1,3699) | 2:1:C:MET:HE3   | 2:3:C:ILE:HD12  | 8                   | 0.53     | 0.58                | 0.34       |
| (1,3699) | 2:1:C:MET:HE2   | 2:3:C:ILE:HD13  | 8                   | 0.53     | 0.58                | 0.34       |
| (1,1840) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 8                   | 0.46     | 0.13                | 0.45       |
| (1,1840) | 2:6:B:LYS:HG2   | 2:66:B:THR:HG23 | 8                   | 0.46     | 0.13                | 0.45       |
| (1,1840) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG23 | 8                   | 0.46     | 0.13                | 0.45       |
| (1,1840) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG21 | 8                   | 0.46     | 0.13                | 0.45       |
| (1,1492) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD12 | 8                   | 0.43     | 0.45                | 0.2        |
| (1,1492) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD13 | 8                   | 0.43     | 0.45                | 0.2        |
| (1,1492) | 2:1:B:MET:HE1   | 2:56:B:LEU:HD11 | 8                   | 0.43     | 0.45                | 0.2        |
| (1,1492) | 2:1:B:MET:HE3   | 2:56:B:LEU:HD13 | 8                   | 0.43     | 0.45                | 0.2        |
| (1,1492) | 2:1:B:MET:HE1   | 2:56:B:LEU:HD13 | 8                   | 0.43     | 0.45                | 0.2        |
| (1,1492) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD11 | 8                   | 0.43     | 0.45                | 0.2        |
| (1,3718) | 2:1:C:MET:HE1   | 2:17:C:VAL:HG21 | 8                   | 0.29     | 0.28                | 0.19       |
| (1,3718) | 2:1:C:MET:HE3   | 2:17:C:VAL:HG22 | 8                   | 0.29     | 0.28                | 0.19       |
| (1,3718) | 2:1:C:MET:HE2   | 2:17:C:VAL:HG21 | 8                   | 0.29     | 0.28                | 0.19       |
| (1,3718) | 2:1:C:MET:HE1   | 2:17:C:VAL:HG23 | 8                   | 0.29     | 0.28                | 0.19       |
| (1,3718) | 2:1:C:MET:HE3   | 2:17:C:VAL:HG21 | 8                   | 0.29     | 0.28                | 0.19       |
| (1,1535) | 2:68:B:HIS:HA   | 2:5:B:VAL:HG13  | 7                   | 0.47     | 0.16                | 0.46       |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,1535) | 2:2:B:GLN:HA     | 2:17:B:VAL:HG12 | 7                   | 0.47     | 0.16                | 0.46       |
| (1,1535) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG12  | 7                   | 0.47     | 0.16                | 0.46       |
| (1,1535) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG11  | 7                   | 0.47     | 0.16                | 0.46       |
| (1,1448) | 2:1:B:MET:HE2    | 2:17:B:VAL:HB   | 7                   | 0.36     | 0.41                | 0.22       |
| (1,1448) | 2:1:B:MET:HE3    | 2:17:B:VAL:HB   | 7                   | 0.36     | 0.41                | 0.22       |
| (1,1448) | 2:1:B:MET:HE1    | 2:17:B:VAL:HB   | 7                   | 0.36     | 0.41                | 0.22       |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD21 | 7                   | 0.32     | 0.15                | 0.3        |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD22 | 7                   | 0.32     | 0.15                | 0.3        |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD23 | 7                   | 0.32     | 0.15                | 0.3        |
| (1,1511) | 2:1:B:MET:HG3    | 2:63:B:LYS:HA   | 7                   | 0.29     | 0.3                 | 0.18       |
| (1,1511) | 2:1:B:MET:HG2    | 2:63:B:LYS:HA   | 7                   | 0.29     | 0.3                 | 0.18       |
| (1,1774) | 2:5:B:VAL:HA     | 2:66:B:THR:HG23 | 7                   | 0.29     | 0.13                | 0.23       |
| (1,1774) | 2:5:B:VAL:HA     | 2:66:B:THR:HG21 | 7                   | 0.29     | 0.13                | 0.23       |
| (1,1774) | 2:5:B:VAL:HA     | 2:66:B:THR:HG22 | 7                   | 0.29     | 0.13                | 0.23       |
| (1,1775) | 2:5:B:VAL:HA     | 2:66:B:THR:HG23 | 7                   | 0.29     | 0.13                | 0.23       |
| (1,1775) | 2:5:B:VAL:HA     | 2:66:B:THR:HG21 | 7                   | 0.29     | 0.13                | 0.23       |
| (1,1775) | 2:5:B:VAL:HA     | 2:66:B:THR:HG22 | 7                   | 0.29     | 0.13                | 0.23       |
| (3,26)   | 2:2:B:GLN:HG2    | 2:3:B:ILE:HA    | 7                   | 0.28     | 0.07                | 0.25       |
| (3,26)   | 2:2:B:GLN:HG3    | 2:3:B:ILE:HA    | 7                   | 0.28     | 0.07                | 0.25       |
| (1,4203) | 2:12:C:THR:HG22  | 2:13:C:ILE:HA   | 7                   | 0.27     | 0.08                | 0.23       |
| (1,4203) | 2:12:C:THR:HG23  | 2:13:C:ILE:HA   | 7                   | 0.27     | 0.08                | 0.23       |
| (1,4203) | 2:12:C:THR:HG21  | 2:13:C:ILE:HA   | 7                   | 0.27     | 0.08                | 0.23       |
| (1,5900) | 2:70:C:VAL:HG13  | 2:68:C:HIS:HB3  | 7                   | 0.25     | 0.14                | 0.2        |
| (1,5900) | 2:66:C:THR:HG22  | 2:68:C:HIS:HB3  | 7                   | 0.25     | 0.14                | 0.2        |
| (1,5900) | 2:70:C:VAL:HG12  | 2:68:C:HIS:HB3  | 7                   | 0.25     | 0.14                | 0.2        |
| (1,5900) | 2:70:C:VAL:HG11  | 2:68:C:HIS:HB3  | 7                   | 0.25     | 0.14                | 0.2        |
| (1,3714) | 2:1:C:MET:HE1    | 2:17:C:VAL:HB   | 7                   | 0.23     | 0.13                | 0.17       |
| (1,3714) | 2:1:C:MET:HE3    | 2:17:C:VAL:HB   | 7                   | 0.23     | 0.13                | 0.17       |
| (1,3714) | 2:1:C:MET:HE2    | 2:17:C:VAL:HB   | 7                   | 0.23     | 0.13                | 0.17       |
| (1,865)  | 1:520:A:ILE:HG12 | 1:562:A:TRP:HZ2 | 6                   | 0.69     | 0.23                | 0.6        |
| (1,865)  | 1:520:A:ILE:HG12 | 1:562:A:TRP:HD1 | 6                   | 0.69     | 0.23                | 0.6        |
| (1,865)  | 1:520:A:ILE:HG13 | 1:562:A:TRP:HD1 | 6                   | 0.69     | 0.23                | 0.6        |
| (1,865)  | 1:520:A:ILE:HG12 | 1:562:A:TRP:HE3 | 6                   | 0.69     | 0.23                | 0.6        |
| (1,865)  | 1:520:A:ILE:HG13 | 1:562:A:TRP:HE3 | 6                   | 0.69     | 0.23                | 0.6        |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD23 | 6                   | 0.68     | 0.3                 | 0.62       |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD21 | 6                   | 0.68     | 0.3                 | 0.62       |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD22 | 6                   | 0.68     | 0.3                 | 0.62       |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD11 | 6                   | 0.68     | 0.3                 | 0.62       |
| (1,3014) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD23 | 6                   | 0.59     | 0.3                 | 0.53       |
| (1,3014) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD21 | 6                   | 0.59     | 0.3                 | 0.53       |
| (1,3014) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD22 | 6                   | 0.59     | 0.3                 | 0.53       |
| (1,3014) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD11 | 6                   | 0.59     | 0.3                 | 0.53       |

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| Key      | Atom-1          | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3854) | 2:29:C:LYS:HA   | 2:15:C:LEU:HD22 | 6                   | 0.44     | 0.16                | 0.42       |
| (1,3854) | 2:29:C:LYS:HA   | 2:15:C:LEU:HD12 | 6                   | 0.44     | 0.16                | 0.42       |
| (1,3854) | 2:29:C:LYS:HA   | 2:15:C:LEU:HD11 | 6                   | 0.44     | 0.16                | 0.42       |
| (1,3854) | 2:29:C:LYS:HA   | 2:15:C:LEU:HD13 | 6                   | 0.44     | 0.16                | 0.42       |
| (1,414)  | 1:547:A:MET:HE1 | 1:548:A:ASP:H   | 6                   | 0.38     | 0.14                | 0.38       |
| (1,414)  | 1:547:A:MET:HE2 | 1:548:A:ASP:H   | 6                   | 0.38     | 0.14                | 0.38       |
| (1,414)  | 1:547:A:MET:HE3 | 1:548:A:ASP:H   | 6                   | 0.38     | 0.14                | 0.38       |
| (1,5279) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD22 | 6                   | 0.38     | 0.18                | 0.45       |
| (1,5279) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD23 | 6                   | 0.38     | 0.18                | 0.45       |
| (1,5279) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD21 | 6                   | 0.38     | 0.18                | 0.45       |
| (1,4339) | 2:15:C:LEU:HD23 | 2:33:C:LYS:HD2  | 6                   | 0.36     | 0.11                | 0.4        |
| (1,4339) | 2:15:C:LEU:HD13 | 2:33:C:LYS:HD2  | 6                   | 0.36     | 0.11                | 0.4        |
| (1,4339) | 2:15:C:LEU:HD12 | 2:33:C:LYS:HD2  | 6                   | 0.36     | 0.11                | 0.4        |
| (1,4339) | 2:15:C:LEU:HD22 | 2:33:C:LYS:HD2  | 6                   | 0.36     | 0.11                | 0.4        |
| (1,5185) | 2:36:C:ILE:HG22 | 2:71:C:LEU:HD22 | 6                   | 0.35     | 0.22                | 0.32       |
| (1,5185) | 2:36:C:ILE:HG23 | 2:71:C:LEU:HD23 | 6                   | 0.35     | 0.22                | 0.32       |
| (1,5185) | 2:36:C:ILE:HG21 | 2:71:C:LEU:HD23 | 6                   | 0.35     | 0.22                | 0.32       |
| (1,1767) | 2:17:B:VAL:HG12 | 2:29:B:LYS:HG3  | 6                   | 0.33     | 0.17                | 0.36       |
| (1,1767) | 2:17:B:VAL:HG13 | 2:29:B:LYS:HG3  | 6                   | 0.33     | 0.17                | 0.36       |
| (1,1767) | 2:17:B:VAL:HG11 | 2:29:B:LYS:HG3  | 6                   | 0.33     | 0.17                | 0.36       |
| (1,3036) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD13 | 6                   | 0.32     | 0.09                | 0.34       |
| (1,3036) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD23 | 6                   | 0.32     | 0.09                | 0.34       |
| (1,3036) | 2:41:B:GLN:HA   | 2:71:B:LEU:HD22 | 6                   | 0.32     | 0.09                | 0.34       |
| (1,3036) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD12 | 6                   | 0.32     | 0.09                | 0.34       |
| (1,3036) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD11 | 6                   | 0.32     | 0.09                | 0.34       |
| (1,3888) | 2:29:C:LYS:HA   | 2:33:C:LYS:HE2  | 6                   | 0.27     | 0.07                | 0.27       |
| (1,3888) | 2:29:C:LYS:HA   | 2:33:C:LYS:HE3  | 6                   | 0.27     | 0.07                | 0.27       |
| (1,1838) | 2:6:B:LYS:HG2   | 2:66:B:THR:HG23 | 6                   | 0.19     | 0.1                 | 0.16       |
| (1,1838) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 6                   | 0.19     | 0.1                 | 0.16       |
| (1,1838) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG23 | 6                   | 0.19     | 0.1                 | 0.16       |
| (1,1838) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG21 | 6                   | 0.19     | 0.1                 | 0.16       |
| (1,3740) | 2:28:C:ALA:HB3  | 2:25:C:ASN:HA   | 6                   | 0.17     | 0.03                | 0.18       |
| (1,3740) | 2:28:C:ALA:HB2  | 2:25:C:ASN:HA   | 6                   | 0.17     | 0.03                | 0.18       |
| (1,3740) | 2:28:C:ALA:HB1  | 2:25:C:ASN:HA   | 6                   | 0.17     | 0.03                | 0.18       |
| (1,407)  | 1:547:A:MET:HE1 | 1:547:A:MET:H   | 6                   | 0.14     | 0.02                | 0.13       |
| (1,407)  | 1:547:A:MET:HE2 | 1:547:A:MET:H   | 6                   | 0.14     | 0.02                | 0.13       |
| (1,407)  | 1:547:A:MET:HE3 | 1:547:A:MET:H   | 6                   | 0.14     | 0.02                | 0.13       |
| (1,75)   | 1:548:A:ASP:OD1 | 2:42:B:ARG:NH2  | 5                   | 1.1      | 0.61                | 1.01       |
| (1,75)   | 1:548:A:ASP:OD2 | 2:42:B:ARG:NH2  | 5                   | 1.1      | 0.61                | 1.01       |
| (1,2073) | 2:15:B:LEU:HD12 | 2:33:B:LYS:HD2  | 5                   | 0.38     | 0.1                 | 0.38       |
| (1,2073) | 2:15:B:LEU:HD23 | 2:33:B:LYS:HD2  | 5                   | 0.38     | 0.1                 | 0.38       |
| (1,2073) | 2:15:B:LEU:HD21 | 2:33:B:LYS:HD2  | 5                   | 0.38     | 0.1                 | 0.38       |

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| Key      | Atom-1          | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|-----------------|------------------|---------------------|----------|---------------------|------------|
| (1,2073) | 2:15:B:LEU:HD22 | 2:33:B:LYS:HD2   | 5                   | 0.38     | 0.1                 | 0.38       |
| (1,3802) | 2:2:C:GLN:HE22  | 2:14:C:THR:HG22  | 5                   | 0.35     | 0.14                | 0.33       |
| (1,3802) | 2:2:C:GLN:HE22  | 2:14:C:THR:HG21  | 5                   | 0.35     | 0.14                | 0.33       |
| (1,3035) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD13  | 5                   | 0.31     | 0.05                | 0.32       |
| (1,3035) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD23  | 5                   | 0.31     | 0.05                | 0.32       |
| (1,3035) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD12  | 5                   | 0.31     | 0.05                | 0.32       |
| (1,3035) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD11  | 5                   | 0.31     | 0.05                | 0.32       |
| (1,3035) | 2:41:B:GLN:HA   | 2:71:B:LEU:HD22  | 5                   | 0.31     | 0.05                | 0.32       |
| (3,146)  | 2:2:C:GLN:HG2   | 2:3:C:ILE:HA     | 5                   | 0.31     | 0.06                | 0.34       |
| (1,1622) | 2:29:B:LYS:HA   | 2:33:B:LYS:HE3   | 5                   | 0.31     | 0.1                 | 0.26       |
| (1,1622) | 2:29:B:LYS:HA   | 2:33:B:LYS:HE2   | 5                   | 0.31     | 0.1                 | 0.26       |
| (1,122)  | 1:503:A:ASP:H   | 1:506:A:LEU:H    | 5                   | 0.23     | 0.08                | 0.21       |
| (1,2919) | 2:36:B:ILE:HG23 | 2:71:B:LEU:HD11  | 4                   | 0.76     | 0.29                | 0.92       |
| (1,2919) | 2:36:B:ILE:HG23 | 2:71:B:LEU:HD13  | 4                   | 0.76     | 0.29                | 0.92       |
| (1,2919) | 2:36:B:ILE:HG21 | 2:71:B:LEU:HD13  | 4                   | 0.76     | 0.29                | 0.92       |
| (1,2919) | 2:36:B:ILE:HG22 | 2:71:B:LEU:HD13  | 4                   | 0.76     | 0.29                | 0.92       |
| (1,1433) | 2:1:B:MET:HE3   | 2:3:B:ILE:HD12   | 4                   | 0.76     | 0.75                | 0.36       |
| (1,1433) | 2:1:B:MET:HE2   | 2:3:B:ILE:HD13   | 4                   | 0.76     | 0.75                | 0.36       |
| (1,1433) | 2:1:B:MET:HE2   | 2:3:B:ILE:HD12   | 4                   | 0.76     | 0.75                | 0.36       |
| (3,24)   | 2:1:B:MET:HE2   | 2:67:B:LEU:HD21  | 4                   | 0.75     | 0.84                | 0.34       |
| (3,24)   | 2:1:B:MET:HE1   | 2:67:B:LEU:HD13  | 4                   | 0.75     | 0.84                | 0.34       |
| (3,24)   | 2:1:B:MET:HE2   | 2:67:B:LEU:HD13  | 4                   | 0.75     | 0.84                | 0.34       |
| (3,24)   | 2:1:B:MET:HE1   | 2:67:B:LEU:HD12  | 4                   | 0.75     | 0.84                | 0.34       |
| (1,3013) | 2:40:B:GLN:HB3  | 2:71:B:LEU:HD22  | 4                   | 0.62     | 0.3                 | 0.72       |
| (1,3013) | 2:40:B:GLN:HB3  | 2:71:B:LEU:HD23  | 4                   | 0.62     | 0.3                 | 0.72       |
| (1,3013) | 2:40:B:GLN:HB3  | 2:71:B:LEU:HD21  | 4                   | 0.62     | 0.3                 | 0.72       |
| (1,1750) | 2:5:B:VAL:HG22  | 2:13:B:ILE:HG13  | 4                   | 0.59     | 0.18                | 0.66       |
| (1,1750) | 2:5:B:VAL:HG22  | 2:15:B:LEU:HG    | 4                   | 0.59     | 0.18                | 0.66       |
| (1,1750) | 2:5:B:VAL:HG23  | 2:15:B:LEU:HG    | 4                   | 0.59     | 0.18                | 0.66       |
| (1,1119) | 1:554:A:THR:HB  | 1:556:A:ILE:HG21 | 4                   | 0.57     | 0.3                 | 0.61       |
| (1,1119) | 1:554:A:THR:HB  | 1:556:A:ILE:HG22 | 4                   | 0.57     | 0.3                 | 0.61       |
| (1,1119) | 1:554:A:THR:HB  | 1:556:A:ILE:HG23 | 4                   | 0.57     | 0.3                 | 0.61       |
| (1,2844) | 2:34:B:GLU:HG3  | 2:69:B:LEU:HD23  | 4                   | 0.55     | 0.27                | 0.62       |
| (1,2844) | 2:34:B:GLU:HG3  | 2:69:B:LEU:HD22  | 4                   | 0.55     | 0.27                | 0.62       |
| (1,2844) | 2:34:B:GLU:HG3  | 2:69:B:LEU:HD21  | 4                   | 0.55     | 0.27                | 0.62       |
| (1,2844) | 2:34:B:GLU:HG3  | 2:69:B:LEU:HD12  | 4                   | 0.55     | 0.27                | 0.62       |
| (3,33)   | 2:3:B:ILE:HG23  | 2:67:B:LEU:HG    | 4                   | 0.53     | 0.18                | 0.6        |
| (3,33)   | 2:3:B:ILE:HG21  | 2:67:B:LEU:HG    | 4                   | 0.53     | 0.18                | 0.6        |
| (3,33)   | 2:3:B:ILE:HG22  | 2:67:B:LEU:HG    | 4                   | 0.53     | 0.18                | 0.6        |
| (1,1748) | 2:5:B:VAL:HG22  | 2:13:B:ILE:HG13  | 4                   | 0.43     | 0.18                | 0.5        |
| (1,1748) | 2:5:B:VAL:HG22  | 2:15:B:LEU:HG    | 4                   | 0.43     | 0.18                | 0.5        |
| (1,1748) | 2:5:B:VAL:HG23  | 2:15:B:LEU:HG    | 4                   | 0.43     | 0.18                | 0.5        |

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| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,4072) | 2:11:C:LYS:HG2   | 2:10:C:GLY:HA3  | 4                   | 0.33     | 0.11                | 0.38       |
| (1,2056) | 2:15:B:LEU:HD13  | 2:29:B:LYS:HG2  | 4                   | 0.33     | 0.24                | 0.22       |
| (1,2056) | 2:15:B:LEU:HD11  | 2:29:B:LYS:HG3  | 4                   | 0.33     | 0.24                | 0.22       |
| (1,2056) | 2:15:B:LEU:HD12  | 2:29:B:LYS:HG2  | 4                   | 0.33     | 0.24                | 0.22       |
| (1,1749) | 2:5:B:VAL:HG22   | 2:13:B:ILE:HG13 | 4                   | 0.21     | 0.05                | 0.22       |
| (1,1749) | 2:5:B:VAL:HG23   | 2:13:B:ILE:HG13 | 4                   | 0.21     | 0.05                | 0.22       |
| (1,4155) | 2:7:C:THR:HB     | 2:69:C:LEU:HD21 | 4                   | 0.2      | 0.04                | 0.2        |
| (1,4155) | 2:7:C:THR:HB     | 2:69:C:LEU:HD23 | 4                   | 0.2      | 0.04                | 0.2        |
| (1,4155) | 2:7:C:THR:HB     | 2:69:C:LEU:HD22 | 4                   | 0.2      | 0.04                | 0.2        |
| (1,5278) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD22 | 4                   | 0.19     | 0.07                | 0.19       |
| (1,5278) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD21 | 4                   | 0.19     | 0.07                | 0.19       |
| (1,5278) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD23 | 4                   | 0.19     | 0.07                | 0.19       |
| (1,1474) | 2:28:B:ALA:HB1   | 2:25:B:ASN:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1474) | 2:28:B:ALA:HB2   | 2:25:B:ASN:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,1474) | 2:28:B:ALA:HB3   | 2:25:B:ASN:HA   | 4                   | 0.14     | 0.03                | 0.14       |
| (1,4107) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21 | 3                   | 1.01     | 0.11                | 1.09       |
| (1,4107) | 2:6:C:LYS:HG2    | 2:66:C:THR:HG21 | 3                   | 1.01     | 0.11                | 1.09       |
| (3,89)   | 2:27:B:LYS:HE2   | 2:69:B:LEU:HD13 | 3                   | 0.88     | 0.63                | 0.87       |
| (3,89)   | 2:27:B:LYS:HE3   | 2:69:B:LEU:HD12 | 3                   | 0.88     | 0.63                | 0.87       |
| (1,263)  | 1:516:A:THR:HA   | 1:518:A:LEU:H   | 3                   | 0.82     | 0.41                | 0.63       |
| (1,258)  | 1:516:A:THR:H    | 1:518:A:LEU:H   | 3                   | 0.75     | 0.39                | 0.58       |
| (1,4105) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21 | 3                   | 0.7      | 0.11                | 0.78       |
| (1,4105) | 2:6:C:LYS:HG2    | 2:66:C:THR:HG21 | 3                   | 0.7      | 0.11                | 0.78       |
| (1,4106) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21 | 3                   | 0.59     | 0.11                | 0.67       |
| (1,4106) | 2:6:C:LYS:HG2    | 2:66:C:THR:HG21 | 3                   | 0.59     | 0.11                | 0.67       |
| (1,2845) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD23 | 3                   | 0.59     | 0.15                | 0.67       |
| (1,2845) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD22 | 3                   | 0.59     | 0.15                | 0.67       |
| (1,2845) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD12 | 3                   | 0.59     | 0.15                | 0.67       |
| (1,1837) | 2:6:B:LYS:HE3    | 2:66:B:THR:HG22 | 3                   | 0.56     | 0.19                | 0.45       |
| (1,1837) | 2:6:B:LYS:HE2    | 2:66:B:THR:HG21 | 3                   | 0.56     | 0.19                | 0.45       |
| (1,1837) | 2:6:B:LYS:HE3    | 2:66:B:THR:HG23 | 3                   | 0.56     | 0.19                | 0.45       |
| (3,139)  | 2:66:B:THR:HG21  | 2:67:B:LEU:HD12 | 3                   | 0.54     | 0.12                | 0.6        |
| (3,139)  | 2:66:B:THR:HG23  | 2:67:B:LEU:HD21 | 3                   | 0.54     | 0.12                | 0.6        |
| (3,139)  | 2:66:B:THR:HG21  | 2:67:B:LEU:HD22 | 3                   | 0.54     | 0.12                | 0.6        |
| (1,2920) | 2:36:B:ILE:HG23  | 2:71:B:LEU:HD11 | 3                   | 0.52     | 0.01                | 0.52       |
| (1,2920) | 2:36:B:ILE:HG23  | 2:71:B:LEU:HD13 | 3                   | 0.52     | 0.01                | 0.52       |
| (1,2920) | 2:36:B:ILE:HG21  | 2:71:B:LEU:HD13 | 3                   | 0.52     | 0.01                | 0.52       |
| (1,3050) | 2:42:B:ARG:HA    | 2:69:B:LEU:HD23 | 3                   | 0.5      | 0.07                | 0.53       |
| (1,3012) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD22 | 3                   | 0.48     | 0.1                 | 0.42       |
| (1,3012) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD23 | 3                   | 0.48     | 0.1                 | 0.42       |
| (1,3012) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD21 | 3                   | 0.48     | 0.1                 | 0.42       |
| (1,73)   | 1:591:A:ILE:HG21 | 2:44:B:ILE:HG22 | 3                   | 0.47     | 0.12                | 0.39       |

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| Key      | Atom-1           | Atom-2           | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|------------------|---------------------|----------|---------------------|------------|
| (1,73)   | 1:591:A:ILE:HG23 | 2:44:B:ILE:HG23  | 3                   | 0.47     | 0.12                | 0.39       |
| (1,73)   | 1:591:A:ILE:HG21 | 2:44:B:ILE:HG23  | 3                   | 0.47     | 0.12                | 0.39       |
| (1,3017) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD22  | 3                   | 0.31     | 0.09                | 0.25       |
| (1,3017) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD23  | 3                   | 0.31     | 0.09                | 0.25       |
| (1,3017) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD21  | 3                   | 0.31     | 0.09                | 0.25       |
| (1,4322) | 2:15:C:LEU:HD12  | 2:29:C:LYS:HG3   | 3                   | 0.31     | 0.08                | 0.32       |
| (1,4322) | 2:15:C:LEU:HD11  | 2:29:C:LYS:HG2   | 3                   | 0.31     | 0.08                | 0.32       |
| (1,4033) | 2:17:C:VAL:HG13  | 2:29:C:LYS:HG3   | 3                   | 0.3      | 0.08                | 0.27       |
| (1,4033) | 2:17:C:VAL:HG12  | 2:29:C:LYS:HG3   | 3                   | 0.3      | 0.08                | 0.27       |
| (1,507)  | 1:575:A:MET:HE1  | 1:575:A:MET:H    | 3                   | 0.29     | 0.15                | 0.3        |
| (1,507)  | 1:575:A:MET:HE2  | 1:575:A:MET:H    | 3                   | 0.29     | 0.15                | 0.3        |
| (1,507)  | 1:575:A:MET:HE3  | 1:575:A:MET:H    | 3                   | 0.29     | 0.15                | 0.3        |
| (1,1836) | 2:6:B:LYS:HD2    | 2:66:B:THR:HG21  | 3                   | 0.28     | 0.08                | 0.25       |
| (1,1836) | 2:6:B:LYS:HD2    | 2:66:B:THR:HG23  | 3                   | 0.28     | 0.08                | 0.25       |
| (1,4205) | 2:12:C:THR:HG21  | 2:13:C:ILE:H     | 3                   | 0.27     | 0.11                | 0.3        |
| (1,4104) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21  | 3                   | 0.27     | 0.11                | 0.34       |
| (1,4104) | 2:6:C:LYS:HG2    | 2:66:C:THR:HG21  | 3                   | 0.27     | 0.11                | 0.34       |
| (1,2924) | 2:36:B:ILE:HG23  | 2:71:B:LEU:HD11  | 3                   | 0.25     | 0.01                | 0.25       |
| (1,2924) | 2:36:B:ILE:HG23  | 2:71:B:LEU:HD13  | 3                   | 0.25     | 0.01                | 0.25       |
| (1,2924) | 2:36:B:ILE:HG21  | 2:71:B:LEU:HD13  | 3                   | 0.25     | 0.01                | 0.25       |
| (1,1559) | 2:68:B:HIS:HA    | 2:66:B:THR:HG23  | 3                   | 0.23     | 0.02                | 0.24       |
| (1,1559) | 2:68:B:HIS:HA    | 2:66:B:THR:HG22  | 3                   | 0.23     | 0.02                | 0.24       |
| (1,4160) | 2:7:C:THR:HG23   | 2:69:C:LEU:HD21  | 3                   | 0.23     | 0.03                | 0.21       |
| (1,4160) | 2:7:C:THR:HG23   | 2:69:C:LEU:HD23  | 3                   | 0.23     | 0.03                | 0.21       |
| (1,4160) | 2:7:C:THR:HG22   | 2:69:C:LEU:HD21  | 3                   | 0.23     | 0.03                | 0.21       |
| (1,1766) | 2:17:B:VAL:HG12  | 2:29:B:LYS:HG3   | 3                   | 0.17     | 0.08                | 0.13       |
| (1,1766) | 2:17:B:VAL:HG13  | 2:29:B:LYS:HG3   | 3                   | 0.17     | 0.08                | 0.13       |
| (1,3644) | 2:67:B:LEU:HB3   | 2:68:B:HIS:H     | 3                   | 0.16     | 0.02                | 0.15       |
| (1,4515) | 2:52:C:ASP:HB2   | 2:24:C:GLU:HB2   | 3                   | 0.1      | 0.0                 | 0.1        |
| (1,4095) | 2:11:C:LYS:HG3   | 2:13:C:ILE:HD13  | 2                   | 1.53     | 0.01                | 1.53       |
| (1,4095) | 2:11:C:LYS:HG3   | 2:13:C:ILE:HD11  | 2                   | 1.53     | 0.01                | 1.53       |
| (1,4096) | 2:11:C:LYS:HG2   | 2:13:C:ILE:HG22  | 2                   | 0.96     | 0.03                | 0.96       |
| (1,4096) | 2:11:C:LYS:HG2   | 2:13:C:ILE:HG21  | 2                   | 0.96     | 0.03                | 0.96       |
| (1,1451) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG21  | 2                   | 0.77     | 0.62                | 0.77       |
| (1,1451) | 2:1:B:MET:HE3    | 2:17:B:VAL:HG22  | 2                   | 0.77     | 0.62                | 0.77       |
| (1,4016) | 2:5:C:VAL:HG23   | 2:13:C:ILE:HG13  | 2                   | 0.72     | 0.02                | 0.72       |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD11 | 2                   | 0.57     | 0.4                 | 0.57       |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD12 | 2                   | 0.57     | 0.4                 | 0.57       |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD13 | 2                   | 0.57     | 0.4                 | 0.57       |
| (1,4014) | 2:5:C:VAL:HG23   | 2:13:C:ILE:HG13  | 2                   | 0.57     | 0.02                | 0.57       |
| (3,209)  | 2:27:C:LYS:HE2   | 2:69:C:LEU:HD13  | 2                   | 0.57     | 0.04                | 0.57       |
| (3,209)  | 2:27:C:LYS:HE2   | 2:69:C:LEU:HD11  | 2                   | 0.57     | 0.04                | 0.57       |

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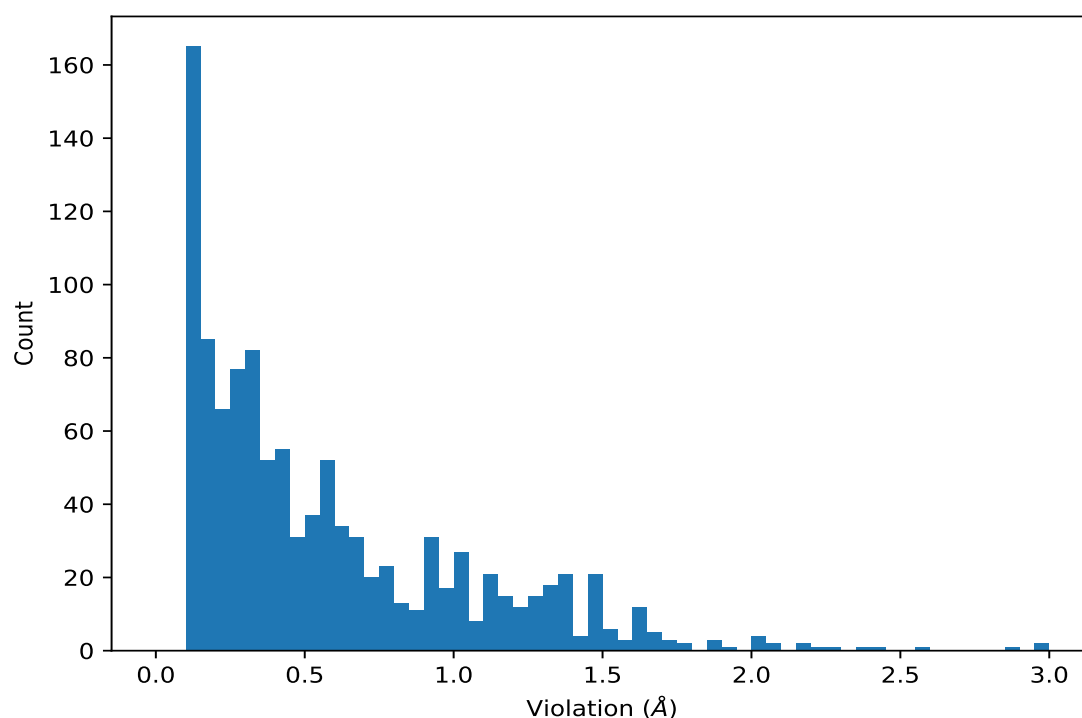
| Key      | Atom-1           | Atom-2          | Models <sup>1</sup> | Mean (Å) | SD <sup>1</sup> (Å) | Median (Å) |
|----------|------------------|-----------------|---------------------|----------|---------------------|------------|
| (1,3039) | 2:41:B:GLN:HB3   | 2:69:B:LEU:HD11 | 2                   | 0.54     | 0.02                | 0.54       |
| (1,3777) | 2:1:C:MET:HG3    | 2:63:C:LYS:HA   | 2                   | 0.53     | 0.38                | 0.53       |
| (1,4232) | 2:13:C:ILE:HG21  | 2:15:C:LEU:HD11 | 2                   | 0.45     | 0.11                | 0.45       |
| (1,4232) | 2:13:C:ILE:HG22  | 2:15:C:LEU:HD22 | 2                   | 0.45     | 0.11                | 0.45       |
| (1,2052) | 2:15:B:LEU:HD13  | 2:29:B:LYS:HA   | 2                   | 0.37     | 0.18                | 0.37       |
| (1,2052) | 2:15:B:LEU:HD11  | 2:29:B:LYS:HA   | 2                   | 0.37     | 0.18                | 0.37       |
| (1,448)  | 1:554:A:THR:HB   | 1:555:A:ALA:H   | 2                   | 0.27     | 0.08                | 0.27       |
| (1,4318) | 2:15:C:LEU:HD12  | 2:29:C:LYS:HA   | 2                   | 0.26     | 0.08                | 0.26       |
| (1,4318) | 2:15:C:LEU:HD11  | 2:29:C:LYS:HA   | 2                   | 0.26     | 0.08                | 0.26       |
| (1,76)   | 1:552:A:GLU:OE2  | 2:42:B:ARG:NH1  | 2                   | 0.25     | 0.15                | 0.25       |
| (1,3019) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD11 | 2                   | 0.24     | 0.08                | 0.24       |
| (1,3019) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD21 | 2                   | 0.24     | 0.08                | 0.24       |
| (1,1135) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HB2 | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1135) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HB3 | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1135) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HB2 | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1135) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HB3 | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1135) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HB2 | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1135) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HB3 | 2                   | 0.23     | 0.09                | 0.23       |
| (1,1534) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG11  | 2                   | 0.18     | 0.01                | 0.18       |
| (1,1534) | 2:2:B:GLN:HA     | 2:17:B:VAL:HG12 | 2                   | 0.18     | 0.01                | 0.18       |
| (1,4015) | 2:5:C:VAL:HG23   | 2:13:C:ILE:HG13 | 2                   | 0.17     | 0.06                | 0.17       |
| (1,4015) | 2:5:C:VAL:HG22   | 2:13:C:ILE:HG13 | 2                   | 0.17     | 0.06                | 0.17       |
| (1,1782) | 2:5:B:VAL:HG11   | 2:69:B:LEU:HB3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,1782) | 2:5:B:VAL:HG13   | 2:69:B:LEU:HB3  | 2                   | 0.16     | 0.01                | 0.16       |
| (1,4313) | 2:15:C:LEU:HD13  | 2:26:C:VAL:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,4313) | 2:43:C:LEU:HD12  | 2:26:C:VAL:HA   | 2                   | 0.12     | 0.02                | 0.12       |
| (1,1783) | 2:5:B:VAL:HG11   | 2:69:B:LEU:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |
| (1,1783) | 2:5:B:VAL:HG13   | 2:69:B:LEU:HB3  | 2                   | 0.11     | 0.0                 | 0.11       |

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

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

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

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



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

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

| Key      | Atom-1         | Atom-2          | Model ID | Violation (Å) |
|----------|----------------|-----------------|----------|---------------|
| (1,3778) | 2:1:C:MET:HE1  | 2:67:C:LEU:HD13 | 1        | 2.97          |
| (1,1450) | 2:1:B:MET:HE2  | 2:17:B:VAL:HG11 | 1        | 2.96          |
| (1,1512) | 2:1:B:MET:HE2  | 2:67:B:LEU:HD21 | 1        | 2.9           |
| (1,1449) | 2:1:B:MET:HE2  | 2:17:B:VAL:HG11 | 1        | 2.58          |
| (1,256)  | 1:515:A:SER:HA | 1:518:A:LEU:H   | 10       | 2.42          |
| (1,3716) | 2:1:C:MET:HE1  | 2:17:C:VAL:HG12 | 1        | 2.4           |
| (3,144)  | 2:1:C:MET:HE1  | 2:67:C:LEU:HD13 | 1        | 2.26          |
| (1,3020) | 2:40:B:GLN:HG2 | 2:71:B:LEU:HD21 | 3        | 2.22          |
| (3,24)   | 2:1:B:MET:HE2  | 2:67:B:LEU:HD21 | 1        | 2.19          |
| (1,256)  | 1:515:A:SER:HA | 1:518:A:LEU:H   | 6        | 2.19          |
| (1,5286) | 2:40:C:GLN:HG2 | 2:71:C:LEU:HD23 | 6        | 2.06          |
| (1,1433) | 2:1:B:MET:HE2  | 2:3:B:ILE:HD13  | 1        | 2.06          |
| (1,3699) | 2:1:C:MET:HE1  | 2:3:C:ILE:HD13  | 1        | 2.05          |
| (1,3020) | 2:40:B:GLN:HG3 | 2:71:B:LEU:HD23 | 1        | 2.03          |
| (1,3715) | 2:1:C:MET:HE1  | 2:17:C:VAL:HG12 | 1        | 2.02          |
| (1,3020) | 2:40:B:GLN:HG3 | 2:71:B:LEU:HD22 | 8        | 2.02          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,5286) | 2:40:C:GLN:HG2   | 2:71:C:LEU:HD22 | 8        | 1.93          |
| (1,5286) | 2:40:C:GLN:HG3   | 2:71:C:LEU:HD23 | 5        | 1.9           |
| (1,75)   | 1:548:A:ASP:OD1  | 2:42:B:ARG:NH2  | 2        | 1.89          |
| (1,1390) | 1:599:A:ILE:HD12 | 1:562:A:TRP:HZ3 | 5        | 1.85          |
| (1,5286) | 2:40:C:GLN:HG2   | 2:71:C:LEU:HD21 | 9        | 1.78          |
| (1,1390) | 1:599:A:ILE:HD12 | 1:562:A:TRP:HZ2 | 7        | 1.78          |
| (1,1493) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD12 | 1        | 1.73          |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 5        | 1.73          |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 1        | 1.72          |
| (1,1242) | 1:579:A:GLU:HG2  | 1:608:A:TYR:HE1 | 5        | 1.69          |
| (1,1242) | 1:579:A:GLU:HG2  | 1:608:A:TYR:HE2 | 5        | 1.69          |
| (1,1242) | 1:579:A:GLU:HG3  | 1:608:A:TYR:HE1 | 5        | 1.69          |
| (1,1242) | 1:579:A:GLU:HG3  | 1:608:A:TYR:HE2 | 5        | 1.69          |
| (3,89)   | 2:27:B:LYS:HE2   | 2:69:B:LEU:HD13 | 6        | 1.66          |
| (3,142)  | 2:1:C:MET:HE3    | 2:61:C:ILE:HD12 | 1        | 1.63          |
| (1,1432) | 2:1:B:MET:HE1    | 2:3:B:ILE:HD11  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE1    | 2:3:B:ILE:HD12  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE1    | 2:3:B:ILE:HD13  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE2    | 2:3:B:ILE:HD11  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE2    | 2:3:B:ILE:HD12  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE2    | 2:3:B:ILE:HD13  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE3    | 2:3:B:ILE:HD11  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE3    | 2:3:B:ILE:HD12  | 1        | 1.61          |
| (1,1432) | 2:1:B:MET:HE3    | 2:3:B:ILE:HD13  | 1        | 1.61          |
| (1,1452) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG21 | 1        | 1.6           |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 4        | 1.6           |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 6        | 1.59          |
| (1,75)   | 1:548:A:ASP:OD1  | 2:42:B:ARG:NH2  | 9        | 1.58          |
| (1,1492) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD12 | 1        | 1.55          |
| (1,4095) | 2:11:C:LYS:HG3   | 2:13:C:ILE:HD13 | 4        | 1.54          |
| (1,1390) | 1:599:A:ILE:HD12 | 1:562:A:TRP:HZ3 | 8        | 1.54          |
| (1,4095) | 2:11:C:LYS:HG3   | 2:13:C:ILE:HD11 | 6        | 1.52          |
| (1,1390) | 1:599:A:ILE:HD12 | 1:562:A:TRP:HZ3 | 6        | 1.52          |
| (1,3020) | 2:40:B:GLN:HG2   | 2:71:B:LEU:HD23 | 10       | 1.51          |
| (1,1450) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG11 | 9        | 1.5           |
| (1,3716) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG13 | 6        | 1.49          |
| (1,3698) | 2:1:C:MET:HE1    | 2:3:C:ILE:HD11  | 1        | 1.49          |
| (1,3698) | 2:1:C:MET:HE1    | 2:3:C:ILE:HD12  | 1        | 1.49          |
| (1,3698) | 2:1:C:MET:HE1    | 2:3:C:ILE:HD13  | 1        | 1.49          |
| (1,3698) | 2:1:C:MET:HE2    | 2:3:C:ILE:HD11  | 1        | 1.49          |
| (1,3698) | 2:1:C:MET:HE2    | 2:3:C:ILE:HD12  | 1        | 1.49          |
| (1,3698) | 2:1:C:MET:HE2    | 2:3:C:ILE:HD13  | 1        | 1.49          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3698) | 2:1:C:MET:HE3    | 2:3:C:ILE:HD11  | 1        | 1.49          |
| (1,3698) | 2:1:C:MET:HE3    | 2:3:C:ILE:HD12  | 1        | 1.49          |
| (1,3698) | 2:1:C:MET:HE3    | 2:3:C:ILE:HD13  | 1        | 1.49          |
| (1,1390) | 1:599:A:ILE:HD13 | 1:562:A:TRP:HZ3 | 2        | 1.49          |
| (1,1435) | 2:1:B:MET:HE1    | 2:3:B:ILE:HG21  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE1    | 2:3:B:ILE:HG22  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE1    | 2:3:B:ILE:HG23  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE2    | 2:3:B:ILE:HG21  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE2    | 2:3:B:ILE:HG22  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE2    | 2:3:B:ILE:HG23  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE3    | 2:3:B:ILE:HG21  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE3    | 2:3:B:ILE:HG22  | 1        | 1.48          |
| (1,1435) | 2:1:B:MET:HE3    | 2:3:B:ILE:HG23  | 1        | 1.48          |
| (1,256)  | 1:515:A:SER:HA   | 1:518:A:LEU:H   | 5        | 1.47          |
| (1,1450) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG11 | 10       | 1.45          |
| (1,5286) | 2:40:C:GLN:HG2   | 2:71:C:LEU:HD22 | 3        | 1.43          |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12 | 9        | 1.41          |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12 | 10       | 1.41          |
| (1,5286) | 2:40:C:GLN:HG2   | 2:71:C:LEU:HD22 | 2        | 1.4           |
| (1,1451) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG21 | 1        | 1.39          |
| (1,1450) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG13 | 4        | 1.39          |
| (1,1241) | 1:579:A:GLU:HG2  | 1:608:A:TYR:HD1 | 5        | 1.39          |
| (1,1241) | 1:579:A:GLU:HG2  | 1:608:A:TYR:HD2 | 5        | 1.39          |
| (1,1241) | 1:579:A:GLU:HG3  | 1:608:A:TYR:HD1 | 5        | 1.39          |
| (1,1241) | 1:579:A:GLU:HG3  | 1:608:A:TYR:HD2 | 5        | 1.39          |
| (1,263)  | 1:516:A:THR:HA   | 1:518:A:LEU:H   | 6        | 1.39          |
| (1,1450) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG13 | 7        | 1.38          |
| (1,3716) | 2:1:C:MET:HE2    | 2:17:C:VAL:HG12 | 4        | 1.37          |
| (1,3701) | 2:1:C:MET:HE1    | 2:3:C:ILE:HG21  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE1    | 2:3:C:ILE:HG22  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE1    | 2:3:C:ILE:HG23  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE2    | 2:3:C:ILE:HG21  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE2    | 2:3:C:ILE:HG22  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE2    | 2:3:C:ILE:HG23  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE3    | 2:3:C:ILE:HG21  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE3    | 2:3:C:ILE:HG22  | 1        | 1.36          |
| (1,3701) | 2:1:C:MET:HE3    | 2:3:C:ILE:HG23  | 1        | 1.36          |
| (1,1448) | 2:1:B:MET:HE2    | 2:17:B:VAL:HB   | 1        | 1.36          |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG11 | 7        | 1.35          |
| (1,3759) | 2:1:C:MET:HE1    | 2:56:C:LEU:HD12 | 1        | 1.34          |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG11 | 5        | 1.34          |
| (1,3020) | 2:40:B:GLN:HG2   | 2:71:B:LEU:HD23 | 7        | 1.34          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1450) | 2:1:B:MET:HE3    | 2:17:B:VAL:HG11 | 5        | 1.33          |
| (1,1450) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG13 | 8        | 1.33          |
| (1,3716) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG12 | 8        | 1.32          |
| (1,1390) | 1:599:A:ILE:HD11 | 1:562:A:TRP:HZ3 | 1        | 1.32          |
| (1,3763) | 2:1:C:MET:HE1    | 2:61:C:ILE:HG21 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE1    | 2:61:C:ILE:HG22 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE1    | 2:61:C:ILE:HG23 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE2    | 2:61:C:ILE:HG21 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE2    | 2:61:C:ILE:HG22 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE2    | 2:61:C:ILE:HG23 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE3    | 2:61:C:ILE:HG21 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE3    | 2:61:C:ILE:HG22 | 1        | 1.31          |
| (1,3763) | 2:1:C:MET:HE3    | 2:61:C:ILE:HG23 | 1        | 1.31          |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12 | 3        | 1.31          |
| (1,1450) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG12 | 2        | 1.3           |
| (1,1450) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG11 | 6        | 1.29          |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 3        | 1.29          |
| (1,258)  | 1:516:A:THR:H    | 1:518:A:LEU:H   | 6        | 1.29          |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 9        | 1.28          |
| (1,3716) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12 | 2        | 1.27          |
| (1,1434) | 2:1:B:MET:HE1    | 2:3:B:ILE:HG21  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE1    | 2:3:B:ILE:HG22  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE1    | 2:3:B:ILE:HG23  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE2    | 2:3:B:ILE:HG21  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE2    | 2:3:B:ILE:HG22  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE2    | 2:3:B:ILE:HG23  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE3    | 2:3:B:ILE:HG21  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE3    | 2:3:B:ILE:HG22  | 1        | 1.27          |
| (1,1434) | 2:1:B:MET:HE3    | 2:3:B:ILE:HG23  | 1        | 1.27          |
| (1,256)  | 1:515:A:SER:HA   | 1:518:A:LEU:H   | 8        | 1.26          |
| (1,1450) | 2:1:B:MET:HE3    | 2:17:B:VAL:HG11 | 3        | 1.24          |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 10       | 1.24          |
| (1,1497) | 2:1:B:MET:HE1    | 2:61:B:ILE:HG21 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE1    | 2:61:B:ILE:HG22 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE1    | 2:61:B:ILE:HG23 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE2    | 2:61:B:ILE:HG21 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE2    | 2:61:B:ILE:HG22 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE2    | 2:61:B:ILE:HG23 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE3    | 2:61:B:ILE:HG21 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE3    | 2:61:B:ILE:HG22 | 1        | 1.23          |
| (1,1497) | 2:1:B:MET:HE3    | 2:61:B:ILE:HG23 | 1        | 1.23          |
| (1,256)  | 1:515:A:SER:HA   | 1:518:A:LEU:H   | 1        | 1.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,865)  | 1:520:A:ILE:HG13 | 1:562:A:TRP:HE3 | 9        | 1.2           |
| (3,22)   | 2:1:B:MET:HE2    | 2:61:B:ILE:HD13 | 1        | 1.19          |
| (1,3634) | 2:66:B:THR:HG22  | 2:68:B:HIS:HB3  | 7        | 1.18          |
| (1,5286) | 2:40:C:GLN:HG2   | 2:71:C:LEU:HD22 | 7        | 1.17          |
| (1,3758) | 2:1:C:MET:HE1    | 2:56:C:LEU:HD12 | 1        | 1.17          |
| (1,3700) | 2:1:C:MET:HE1    | 2:3:C:ILE:HG21  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE1    | 2:3:C:ILE:HG22  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE1    | 2:3:C:ILE:HG23  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE2    | 2:3:C:ILE:HG21  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE2    | 2:3:C:ILE:HG22  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE2    | 2:3:C:ILE:HG23  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE3    | 2:3:C:ILE:HG21  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE3    | 2:3:C:ILE:HG22  | 1        | 1.16          |
| (1,3700) | 2:1:C:MET:HE3    | 2:3:C:ILE:HG23  | 1        | 1.16          |
| (1,3634) | 2:70:B:VAL:HG13  | 2:68:B:HIS:HB3  | 10       | 1.16          |
| (1,3762) | 2:1:C:MET:HE1    | 2:61:C:ILE:HB   | 1        | 1.15          |
| (1,3762) | 2:1:C:MET:HE2    | 2:61:C:ILE:HB   | 1        | 1.15          |
| (1,3762) | 2:1:C:MET:HE3    | 2:61:C:ILE:HB   | 1        | 1.15          |
| (1,1841) | 2:6:B:LYS:HG2    | 2:66:B:THR:HG23 | 2        | 1.15          |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H   | 7        | 1.14          |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD21 | 3        | 1.13          |
| (1,1512) | 2:1:B:MET:HE1    | 2:67:B:LEU:HD12 | 7        | 1.13          |
| (1,3764) | 2:1:C:MET:HE1    | 2:61:C:ILE:HG21 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE1    | 2:61:C:ILE:HG22 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE1    | 2:61:C:ILE:HG23 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE2    | 2:61:C:ILE:HG21 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE2    | 2:61:C:ILE:HG22 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE2    | 2:61:C:ILE:HG23 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE3    | 2:61:C:ILE:HG21 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE3    | 2:61:C:ILE:HG22 | 1        | 1.12          |
| (1,3764) | 2:1:C:MET:HE3    | 2:61:C:ILE:HG23 | 1        | 1.12          |
| (1,1449) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG11 | 9        | 1.12          |
| (1,1390) | 1:599:A:ILE:HD11 | 1:562:A:TRP:HZ2 | 4        | 1.12          |
| (1,5281) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD23 | 4        | 1.11          |
| (1,3715) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG13 | 6        | 1.11          |
| (1,3634) | 2:70:B:VAL:HG12  | 2:68:B:HIS:HB3  | 4        | 1.1           |
| (1,4107) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21 | 2        | 1.09          |
| (1,4107) | 2:6:C:LYS:HG2    | 2:66:C:THR:HG21 | 4        | 1.09          |
| (1,256)  | 1:515:A:SER:HA   | 1:518:A:LEU:H   | 9        | 1.08          |
| (1,3045) | 2:41:B:GLN:H     | 2:69:B:LEU:HD23 | 2        | 1.07          |
| (1,1449) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG11 | 10       | 1.07          |
| (1,1505) | 2:1:B:MET:HE1    | 2:63:B:LYS:HA   | 1        | 1.05          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1505) | 2:1:B:MET:HE2    | 2:63:B:LYS:HA    | 1        | 1.05          |
| (1,1505) | 2:1:B:MET:HE3    | 2:63:B:LYS:HA    | 1        | 1.05          |
| (2,4)    | 1:484:A:LYS:O    | 1:488:A:ALA:N    | 3        | 1.04          |
| (1,5286) | 2:40:C:GLN:HG3   | 2:71:C:LEU:HD22  | 1        | 1.04          |
| (1,3014) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD21  | 3        | 1.04          |
| (1,1498) | 2:1:B:MET:HE1    | 2:61:B:ILE:HG21  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE1    | 2:61:B:ILE:HG22  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE1    | 2:61:B:ILE:HG23  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE2    | 2:61:B:ILE:HG21  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE2    | 2:61:B:ILE:HG22  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE2    | 2:61:B:ILE:HG23  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE3    | 2:61:B:ILE:HG21  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE3    | 2:61:B:ILE:HG22  | 1        | 1.04          |
| (1,1498) | 2:1:B:MET:HE3    | 2:61:B:ILE:HG23  | 1        | 1.04          |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12  | 9        | 1.03          |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12  | 10       | 1.03          |
| (1,3634) | 2:66:B:THR:HG21  | 2:68:B:HIS:HB3   | 6        | 1.03          |
| (1,1511) | 2:1:B:MET:HG3    | 2:63:B:LYS:HA    | 1        | 1.03          |
| (1,1506) | 2:1:B:MET:HE1    | 2:63:B:LYS:HA    | 1        | 1.03          |
| (1,1506) | 2:1:B:MET:HE2    | 2:63:B:LYS:HA    | 1        | 1.03          |
| (1,1506) | 2:1:B:MET:HE3    | 2:63:B:LYS:HA    | 1        | 1.03          |
| (1,5280) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD23  | 4        | 1.02          |
| (1,3718) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG21  | 1        | 1.02          |
| (1,3634) | 2:66:B:THR:HG23  | 2:68:B:HIS:HB3   | 3        | 1.02          |
| (1,3634) | 2:66:B:THR:HG21  | 2:68:B:HIS:HB3   | 8        | 1.02          |
| (1,500)  | 1:573:A:LEU:H    | 1:575:A:MET:H    | 2        | 1.02          |
| (1,1449) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG13  | 4        | 1.01          |
| (1,75)   | 1:548:A:ASP:OD2  | 2:42:B:ARG:NH2   | 5        | 1.01          |
| (1,1449) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG13  | 7        | 1.0           |
| (1,4096) | 2:11:C:LYS:HG2   | 2:13:C:ILE:HG21  | 6        | 0.99          |
| (1,3715) | 2:1:C:MET:HE2    | 2:17:C:VAL:HG12  | 4        | 0.99          |
| (1,1390) | 1:599:A:ILE:HD13 | 1:562:A:TRP:HZ2  | 3        | 0.99          |
| (1,5311) | 2:41:C:GLN:H     | 2:71:C:LEU:HD21  | 7        | 0.98          |
| (1,3634) | 2:66:B:THR:HG21  | 2:68:B:HIS:HB3   | 5        | 0.98          |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD11  | 9        | 0.98          |
| (1,1512) | 2:1:B:MET:HE2    | 2:67:B:LEU:HD13  | 6        | 0.98          |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD11 | 1        | 0.98          |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD12 | 1        | 0.98          |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD13 | 1        | 0.98          |
| (2,3)    | 1:484:A:LYS:O    | 1:488:A:ALA:H    | 3        | 0.97          |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG11  | 7        | 0.97          |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG11  | 5        | 0.96          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1841) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG23  | 6        | 0.96          |
| (1,1496) | 2:1:B:MET:HE1    | 2:61:B:ILE:HB    | 1        | 0.96          |
| (1,1496) | 2:1:B:MET:HE2    | 2:61:B:ILE:HB    | 1        | 0.96          |
| (1,1496) | 2:1:B:MET:HE3    | 2:61:B:ILE:HB    | 1        | 0.96          |
| (1,3715) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG12  | 8        | 0.95          |
| (1,2919) | 2:36:B:ILE:HG23  | 2:71:B:LEU:HD11  | 8        | 0.95          |
| (1,1449) | 2:1:B:MET:HE3    | 2:17:B:VAL:HG11  | 5        | 0.95          |
| (1,1449) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG13  | 8        | 0.95          |
| (1,4096) | 2:11:C:LYS:HG2   | 2:13:C:ILE:HG22  | 4        | 0.94          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG21 | 9        | 0.94          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG22 | 9        | 0.94          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG23 | 9        | 0.94          |
| (3,259)  | 2:66:C:THR:HG21  | 2:67:C:LEU:HD22  | 5        | 0.93          |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12  | 3        | 0.93          |
| (1,3013) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD21  | 3        | 0.93          |
| (1,2919) | 2:36:B:ILE:HG23  | 2:71:B:LEU:HD13  | 1        | 0.93          |
| (1,1841) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22  | 3        | 0.93          |
| (1,1588) | 2:29:B:LYS:HA    | 2:15:B:LEU:HD11  | 4        | 0.93          |
| (1,1449) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG12  | 2        | 0.93          |
| (1,3771) | 2:1:C:MET:HE1    | 2:63:C:LYS:HA    | 1        | 0.92          |
| (1,3771) | 2:1:C:MET:HE2    | 2:63:C:LYS:HA    | 1        | 0.92          |
| (1,3771) | 2:1:C:MET:HE3    | 2:63:C:LYS:HA    | 1        | 0.92          |
| (3,259)  | 2:66:C:THR:HG23  | 2:67:C:LEU:HD12  | 9        | 0.91          |
| (1,3777) | 2:1:C:MET:HG3    | 2:63:C:LYS:HA    | 1        | 0.91          |
| (1,2919) | 2:36:B:ILE:HG21  | 2:71:B:LEU:HD13  | 3        | 0.91          |
| (1,1449) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG11  | 6        | 0.91          |
| (1,255)  | 1:515:A:SER:HA   | 1:517:A:ASP:H    | 10       | 0.91          |
| (1,3772) | 2:1:C:MET:HE1    | 2:63:C:LYS:HA    | 1        | 0.9           |
| (1,3772) | 2:1:C:MET:HE2    | 2:63:C:LYS:HA    | 1        | 0.9           |
| (1,3772) | 2:1:C:MET:HE3    | 2:63:C:LYS:HA    | 1        | 0.9           |
| (1,3020) | 2:40:B:GLN:HG2   | 2:71:B:LEU:HD21  | 5        | 0.9           |
| (1,473)  | 1:556:A:ILE:HD11 | 1:555:A:ALA:H    | 1        | 0.9           |
| (1,473)  | 1:556:A:ILE:HD12 | 1:555:A:ALA:H    | 1        | 0.9           |
| (1,473)  | 1:556:A:ILE:HD13 | 1:555:A:ALA:H    | 1        | 0.9           |
| (1,75)   | 1:548:A:ASP:OD1  | 2:42:B:ARG:NH2   | 3        | 0.9           |
| (1,3715) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG12  | 2        | 0.89          |
| (1,3014) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD11  | 9        | 0.89          |
| (1,3634) | 2:70:B:VAL:HG12  | 2:68:B:HIS:HB3   | 9        | 0.88          |
| (1,1841) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22  | 9        | 0.88          |
| (3,89)   | 2:27:B:LYS:HE3   | 2:69:B:LEU:HD12  | 2        | 0.87          |
| (2,4)    | 1:484:A:LYS:O    | 1:488:A:ALA:N    | 5        | 0.86          |
| (1,4107) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21  | 3        | 0.86          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3020) | 2:40:B:GLN:HG3  | 2:71:B:LEU:HD11 | 9        | 0.86          |
| (1,1841) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 4        | 0.86          |
| (1,1841) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG21 | 10       | 0.86          |
| (1,1449) | 2:1:B:MET:HE3   | 2:17:B:VAL:HG11 | 3        | 0.86          |
| (1,5311) | 2:41:C:GLN:H    | 2:69:C:LEU:HD12 | 9        | 0.85          |
| (1,5281) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD22 | 8        | 0.85          |
| (1,1512) | 2:1:B:MET:HE1   | 2:67:B:LEU:HD13 | 9        | 0.85          |
| (1,5281) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD21 | 9        | 0.84          |
| (1,1493) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD12 | 2        | 0.84          |
| (1,5311) | 2:41:C:GLN:H    | 2:69:C:LEU:HD13 | 5        | 0.83          |
| (1,1839) | 2:6:B:LYS:HG2   | 2:66:B:THR:HG23 | 2        | 0.83          |
| (1,1837) | 2:6:B:LYS:HE2   | 2:66:B:THR:HG21 | 3        | 0.82          |
| (1,5185) | 2:36:C:ILE:HG23 | 2:71:C:LEU:HD23 | 4        | 0.81          |
| (1,3717) | 2:1:C:MET:HE1   | 2:17:C:VAL:HG21 | 1        | 0.81          |
| (1,2844) | 2:34:B:GLU:HG3  | 2:69:B:LEU:HD12 | 4        | 0.81          |
| (1,1841) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 1        | 0.81          |
| (1,1512) | 2:1:B:MET:HE1   | 2:67:B:LEU:HD12 | 2        | 0.81          |
| (1,5281) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD22 | 3        | 0.79          |
| (1,3778) | 2:1:C:MET:HE3   | 2:67:C:LEU:HD12 | 3        | 0.79          |
| (1,1479) | 2:1:B:MET:HE1   | 2:26:B:VAL:HG21 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE1   | 2:26:B:VAL:HG22 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE1   | 2:26:B:VAL:HG23 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE2   | 2:26:B:VAL:HG21 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE2   | 2:26:B:VAL:HG22 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE2   | 2:26:B:VAL:HG23 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE3   | 2:26:B:VAL:HG21 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE3   | 2:26:B:VAL:HG22 | 1        | 0.79          |
| (1,1479) | 2:1:B:MET:HE3   | 2:26:B:VAL:HG23 | 1        | 0.79          |
| (1,5311) | 2:41:C:GLN:H    | 2:69:C:LEU:HD11 | 6        | 0.78          |
| (1,4105) | 2:6:C:LYS:HG3   | 2:66:C:THR:HG21 | 2        | 0.78          |
| (1,4105) | 2:6:C:LYS:HG2   | 2:66:C:THR:HG21 | 4        | 0.78          |
| (1,256)  | 1:515:A:SER:HA  | 1:518:A:LEU:H   | 7        | 0.78          |
| (1,2844) | 2:34:B:GLU:HG3  | 2:69:B:LEU:HD22 | 9        | 0.77          |
| (1,5280) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD22 | 8        | 0.76          |
| (1,3759) | 2:1:C:MET:HE1   | 2:56:C:LEU:HD13 | 8        | 0.76          |
| (2,3)    | 1:484:A:LYS:O   | 1:488:A:ALA:H   | 5        | 0.75          |
| (1,5280) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD21 | 9        | 0.75          |
| (1,1750) | 2:5:B:VAL:HG22  | 2:13:B:ILE:HG13 | 1        | 0.75          |
| (1,1750) | 2:5:B:VAL:HG23  | 2:15:B:LEU:HG   | 7        | 0.75          |
| (1,1512) | 2:1:B:MET:HE2   | 2:67:B:LEU:HD11 | 10       | 0.75          |
| (1,5311) | 2:41:C:GLN:H    | 2:69:C:LEU:HD13 | 4        | 0.74          |
| (1,4016) | 2:5:C:VAL:HG23  | 2:13:C:ILE:HG13 | 4        | 0.74          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2056) | 2:15:B:LEU:HD11  | 2:29:B:LYS:HG3  | 4        | 0.74          |
| (1,472)  | 1:556:A:ILE:HG21 | 1:555:A:ALA:H   | 9        | 0.74          |
| (1,472)  | 1:556:A:ILE:HG22 | 1:555:A:ALA:H   | 9        | 0.74          |
| (1,472)  | 1:556:A:ILE:HG23 | 1:555:A:ALA:H   | 9        | 0.74          |
| (1,5311) | 2:41:C:GLN:H     | 2:71:C:LEU:HD22 | 1        | 0.73          |
| (1,5309) | 2:41:C:GLN:HG2   | 2:69:C:LEU:HD11 | 7        | 0.73          |
| (1,3013) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD22 | 8        | 0.73          |
| (2,4)    | 1:484:A:LYS:O    | 1:488:A:ALA:N   | 8        | 0.72          |
| (1,5307) | 2:41:C:GLN:HG2   | 2:69:C:LEU:HD11 | 7        | 0.72          |
| (1,5286) | 2:40:C:GLN:HG3   | 2:71:C:LEU:HD23 | 4        | 0.72          |
| (1,1840) | 2:6:B:LYS:HG2    | 2:66:B:THR:HG23 | 2        | 0.72          |
| (1,256)  | 1:515:A:SER:HA   | 1:518:A:LEU:H   | 4        | 0.72          |
| (3,259)  | 2:66:C:THR:HG22  | 2:67:C:LEU:HD21 | 3        | 0.71          |
| (1,4016) | 2:5:C:VAL:HG23   | 2:13:C:ILE:HG13 | 2        | 0.71          |
| (1,3854) | 2:29:C:LYS:HA    | 2:15:C:LEU:HD12 | 8        | 0.71          |
| (1,3634) | 2:66:B:THR:HG23  | 2:68:B:HIS:HB3  | 2        | 0.71          |
| (1,3013) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD23 | 1        | 0.71          |
| (1,2845) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD12 | 4        | 0.71          |
| (3,259)  | 2:66:C:THR:HG21  | 2:67:C:LEU:HD22 | 10       | 0.7           |
| (3,33)   | 2:3:B:ILE:HG23   | 2:67:B:LEU:HG   | 1        | 0.7           |
| (2,4)    | 1:484:A:LYS:O    | 1:488:A:ALA:N   | 9        | 0.7           |
| (1,5280) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD22 | 3        | 0.7           |
| (3,33)   | 2:3:B:ILE:HG22   | 2:67:B:LEU:HG   | 7        | 0.69          |
| (1,3778) | 2:1:C:MET:HE3    | 2:67:C:LEU:HD11 | 8        | 0.69          |
| (1,3634) | 2:66:B:THR:HG23  | 2:68:B:HIS:HB3  | 1        | 0.69          |
| (1,1535) | 2:2:B:GLN:HA     | 2:17:B:VAL:HG12 | 2        | 0.69          |
| (2,4)    | 1:484:A:LYS:O    | 1:488:A:ALA:N   | 1        | 0.68          |
| (1,4103) | 2:6:C:LYS:HE2    | 2:66:C:THR:HG22 | 10       | 0.68          |
| (1,3833) | 2:3:C:ILE:HD13   | 2:3:C:ILE:HA    | 10       | 0.68          |
| (1,865)  | 1:520:A:ILE:HG12 | 1:562:A:TRP:HZ2 | 2        | 0.68          |
| (1,4106) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21 | 2        | 0.67          |
| (1,4106) | 2:6:C:LYS:HG2    | 2:66:C:THR:HG21 | 4        | 0.67          |
| (1,3833) | 2:3:C:ILE:HD13   | 2:3:C:ILE:HA    | 3        | 0.67          |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD11 | 7        | 0.67          |
| (1,2845) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD22 | 9        | 0.67          |
| (1,1535) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG11  | 8        | 0.67          |
| (1,1492) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD12 | 2        | 0.67          |
| (3,259)  | 2:66:C:THR:HG21  | 2:67:C:LEU:HD21 | 4        | 0.66          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG11  | 9        | 0.66          |
| (1,3045) | 2:41:B:GLN:H     | 2:69:B:LEU:HD13 | 1        | 0.66          |
| (1,1567) | 2:3:B:ILE:HD12   | 2:3:B:ILE:HA    | 5        | 0.66          |
| (3,139)  | 2:66:B:THR:HG21  | 2:67:B:LEU:HD12 | 8        | 0.65          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,3833) | 2:3:C:ILE:HD13   | 2:3:C:ILE:HA     | 1        | 0.65          |
| (1,3833) | 2:3:C:ILE:HD11   | 2:3:C:ILE:HA     | 5        | 0.65          |
| (1,3833) | 2:3:C:ILE:HD13   | 2:3:C:ILE:HA     | 9        | 0.65          |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD22  | 9        | 0.65          |
| (1,1567) | 2:3:B:ILE:HD13   | 2:3:B:ILE:HA     | 3        | 0.65          |
| (1,1567) | 2:3:B:ILE:HD11   | 2:3:B:ILE:HA     | 10       | 0.65          |
| (1,73)   | 1:591:A:ILE:HG21 | 2:44:B:ILE:HG23  | 7        | 0.65          |
| (1,3833) | 2:3:C:ILE:HD12   | 2:3:C:ILE:HA     | 7        | 0.64          |
| (1,3833) | 2:3:C:ILE:HD12   | 2:3:C:ILE:HA     | 8        | 0.64          |
| (1,3045) | 2:41:B:GLN:H     | 2:69:B:LEU:HD12  | 8        | 0.64          |
| (1,3045) | 2:41:B:GLN:H     | 2:69:B:LEU:HD11  | 9        | 0.64          |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD23  | 1        | 0.64          |
| (1,1841) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG21  | 7        | 0.64          |
| (1,1839) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG23  | 6        | 0.64          |
| (1,1567) | 2:3:B:ILE:HD13   | 2:3:B:ILE:HA     | 6        | 0.64          |
| (1,1567) | 2:3:B:ILE:HD12   | 2:3:B:ILE:HA     | 8        | 0.64          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG21 | 3        | 0.64          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG22 | 3        | 0.64          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG23 | 3        | 0.64          |
| (1,3759) | 2:1:C:MET:HE3    | 2:56:C:LEU:HD12  | 7        | 0.63          |
| (1,3745) | 2:1:C:MET:HE1    | 2:26:C:VAL:HG21  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE1    | 2:26:C:VAL:HG22  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE1    | 2:26:C:VAL:HG23  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE2    | 2:26:C:VAL:HG21  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE2    | 2:26:C:VAL:HG22  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE2    | 2:26:C:VAL:HG23  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE3    | 2:26:C:VAL:HG21  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE3    | 2:26:C:VAL:HG22  | 1        | 0.63          |
| (1,3745) | 2:1:C:MET:HE3    | 2:26:C:VAL:HG23  | 1        | 0.63          |
| (1,1567) | 2:3:B:ILE:HD12   | 2:3:B:ILE:HA     | 4        | 0.63          |
| (1,1512) | 2:1:B:MET:HE3    | 2:67:B:LEU:HD13  | 8        | 0.63          |
| (1,1495) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD12  | 1        | 0.63          |
| (1,263)  | 1:516:A:THR:HA   | 1:518:A:LEU:H    | 5        | 0.63          |
| (3,259)  | 2:66:C:THR:HG22  | 2:67:C:LEU:HD21  | 7        | 0.62          |
| (1,5302) | 2:41:C:GLN:HA    | 2:71:C:LEU:HD21  | 1        | 0.62          |
| (1,3012) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD21  | 3        | 0.62          |
| (3,209)  | 2:27:C:LYS:HE2   | 2:69:C:LEU:HD13  | 1        | 0.61          |
| (2,3)    | 1:484:A:LYS:O    | 1:488:A:ALA:H    | 8        | 0.61          |
| (1,3759) | 2:1:C:MET:HE3    | 2:56:C:LEU:HD13  | 10       | 0.61          |
| (1,1839) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22  | 3        | 0.61          |
| (1,865)  | 1:520:A:ILE:HG12 | 1:562:A:TRP:HZ2  | 1        | 0.61          |
| (3,139)  | 2:66:B:THR:HG23  | 2:67:B:LEU:HD21  | 3        | 0.6           |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,5279) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD23  | 6        | 0.6           |
| (1,3833) | 2:3:C:ILE:HD11   | 2:3:C:ILE:HA     | 6        | 0.6           |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD22  | 8        | 0.6           |
| (1,5281) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD22  | 7        | 0.59          |
| (1,4014) | 2:5:C:VAL:HG23   | 2:13:C:ILE:HG13  | 4        | 0.59          |
| (1,3833) | 2:3:C:ILE:HD12   | 2:3:C:ILE:HA     | 4        | 0.59          |
| (1,1767) | 2:17:B:VAL:HG13  | 2:29:B:LYS:HG3   | 3        | 0.59          |
| (1,1748) | 2:5:B:VAL:HG22   | 2:13:B:ILE:HG13  | 1        | 0.59          |
| (1,1748) | 2:5:B:VAL:HG23   | 2:15:B:LEU:HG    | 7        | 0.59          |
| (1,1567) | 2:3:B:ILE:HD11   | 2:3:B:ILE:HA     | 1        | 0.59          |
| (1,1567) | 2:3:B:ILE:HD11   | 2:3:B:ILE:HA     | 9        | 0.59          |
| (1,865)  | 1:520:A:ILE:HG12 | 1:562:A:TRP:HD1  | 3        | 0.59          |
| (1,5311) | 2:41:C:GLN:H     | 2:69:C:LEU:HD11  | 8        | 0.58          |
| (1,5301) | 2:41:C:GLN:HA    | 2:71:C:LEU:HD21  | 1        | 0.58          |
| (1,3833) | 2:3:C:ILE:HD13   | 2:3:C:ILE:HA     | 2        | 0.58          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG11   | 7        | 0.58          |
| (1,3758) | 2:1:C:MET:HE1    | 2:56:C:LEU:HD13  | 8        | 0.58          |
| (1,3045) | 2:41:B:GLN:H     | 2:69:B:LEU:HD11  | 7        | 0.58          |
| (1,3020) | 2:40:B:GLN:HG3   | 2:71:B:LEU:HD22  | 4        | 0.58          |
| (1,1567) | 2:3:B:ILE:HD13   | 2:3:B:ILE:HA     | 7        | 0.58          |
| (1,1512) | 2:1:B:MET:HE3    | 2:67:B:LEU:HD11  | 5        | 0.58          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG21 | 5        | 0.58          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG22 | 5        | 0.58          |
| (1,1119) | 1:554:A:THR:HB   | 1:556:A:ILE:HG23 | 5        | 0.58          |
| (1,474)  | 1:556:A:ILE:HG21 | 1:554:A:THR:H    | 3        | 0.58          |
| (1,474)  | 1:556:A:ILE:HG22 | 1:554:A:THR:H    | 3        | 0.58          |
| (1,474)  | 1:556:A:ILE:HG23 | 1:554:A:THR:H    | 3        | 0.58          |
| (1,258)  | 1:516:A:THR:H    | 1:518:A:LEU:H    | 5        | 0.58          |
| (2,3)    | 1:484:A:LYS:O    | 1:488:A:ALA:H    | 9        | 0.57          |
| (1,3754) | 2:1:C:MET:HE1    | 2:56:C:LEU:HB3   | 1        | 0.57          |
| (1,3050) | 2:42:B:ARG:HA    | 2:69:B:LEU:HD23  | 6        | 0.57          |
| (1,3039) | 2:41:B:GLN:HB3   | 2:69:B:LEU:HD11  | 4        | 0.57          |
| (1,1839) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22  | 9        | 0.57          |
| (1,1750) | 2:5:B:VAL:HG22   | 2:15:B:LEU:HG    | 5        | 0.57          |
| (1,1588) | 2:29:B:LYS:HA    | 2:15:B:LEU:HD13  | 2        | 0.57          |
| (1,3854) | 2:29:C:LYS:HA    | 2:15:C:LEU:HD11  | 7        | 0.56          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG11   | 8        | 0.56          |
| (1,1567) | 2:3:B:ILE:HD11   | 2:3:B:ILE:HA     | 2        | 0.56          |
| (1,865)  | 1:520:A:ILE:HG13 | 1:562:A:TRP:HD1  | 4        | 0.56          |
| (1,414)  | 1:547:A:MET:HE1  | 1:548:A:ASP:H    | 2        | 0.56          |
| (1,414)  | 1:547:A:MET:HE2  | 1:548:A:ASP:H    | 2        | 0.56          |
| (1,414)  | 1:547:A:MET:HE3  | 1:548:A:ASP:H    | 2        | 0.56          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (3,259)  | 2:66:C:THR:HG21 | 2:67:C:LEU:HD23 | 1        | 0.55          |
| (2,3)    | 1:484:A:LYS:O   | 1:488:A:ALA:H   | 1        | 0.55          |
| (1,4232) | 2:13:C:ILE:HG22 | 2:15:C:LEU:HD22 | 6        | 0.55          |
| (1,4014) | 2:5:C:VAL:HG23  | 2:13:C:ILE:HG13 | 2        | 0.55          |
| (1,3802) | 2:2:C:GLN:HE22  | 2:14:C:THR:HG22 | 6        | 0.55          |
| (1,3014) | 2:40:B:GLN:HB2  | 2:71:B:LEU:HD23 | 1        | 0.55          |
| (1,2052) | 2:15:B:LEU:HD11 | 2:29:B:LYS:HA   | 4        | 0.55          |
| (1,1839) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 4        | 0.55          |
| (1,1839) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG21 | 10       | 0.55          |
| (1,4105) | 2:6:C:LYS:HG3   | 2:66:C:THR:HG21 | 3        | 0.54          |
| (1,3714) | 2:1:C:MET:HE1   | 2:17:C:VAL:HB   | 1        | 0.54          |
| (1,1512) | 2:1:B:MET:HE3   | 2:67:B:LEU:HD11 | 3        | 0.54          |
| (3,209)  | 2:27:C:LYS:HE2  | 2:69:C:LEU:HD11 | 4        | 0.53          |
| (1,5362) | 2:43:C:LEU:HD22 | 2:67:C:LEU:HB3  | 1        | 0.53          |
| (1,5281) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD22 | 1        | 0.53          |
| (1,3755) | 2:1:C:MET:HE1   | 2:56:C:LEU:HB3  | 1        | 0.53          |
| (1,3050) | 2:42:B:ARG:HA   | 2:69:B:LEU:HD23 | 2        | 0.53          |
| (1,2920) | 2:36:B:ILE:HG23 | 2:71:B:LEU:HD11 | 8        | 0.53          |
| (1,2073) | 2:15:B:LEU:HD12 | 2:33:B:LYS:HD2  | 10       | 0.53          |
| (1,1840) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG23 | 6        | 0.53          |
| (1,1806) | 2:6:B:LYS:HG2   | 2:10:B:GLY:HA2  | 5        | 0.53          |
| (1,414)  | 1:547:A:MET:HE1 | 1:548:A:ASP:H   | 7        | 0.53          |
| (1,414)  | 1:547:A:MET:HE2 | 1:548:A:ASP:H   | 7        | 0.53          |
| (1,414)  | 1:547:A:MET:HE3 | 1:548:A:ASP:H   | 7        | 0.53          |
| (2,4)    | 1:484:A:LYS:O   | 1:488:A:ALA:N   | 4        | 0.52          |
| (1,4339) | 2:15:C:LEU:HD22 | 2:33:C:LYS:HD2  | 8        | 0.52          |
| (1,3039) | 2:41:B:GLN:HB3  | 2:69:B:LEU:HD11 | 6        | 0.52          |
| (1,2920) | 2:36:B:ILE:HG23 | 2:71:B:LEU:HD13 | 1        | 0.52          |
| (1,500)  | 1:573:A:LEU:H   | 1:575:A:MET:H   | 8        | 0.52          |
| (1,5311) | 2:41:C:GLN:H    | 2:69:C:LEU:HD11 | 10       | 0.51          |
| (1,5279) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD23 | 5        | 0.51          |
| (1,4041) | 2:5:C:VAL:HA    | 2:66:C:THR:HG21 | 10       | 0.51          |
| (1,4040) | 2:5:C:VAL:HA    | 2:66:C:THR:HG21 | 10       | 0.51          |
| (1,3759) | 2:1:C:MET:HE1   | 2:56:C:LEU:HD12 | 3        | 0.51          |
| (1,3014) | 2:40:B:GLN:HB2  | 2:71:B:LEU:HD22 | 8        | 0.51          |
| (3,33)   | 2:3:B:ILE:HG21  | 2:67:B:LEU:HG   | 2        | 0.5           |
| (1,5280) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD22 | 7        | 0.5           |
| (1,2920) | 2:36:B:ILE:HG21 | 2:71:B:LEU:HD13 | 3        | 0.5           |
| (1,1840) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 3        | 0.5           |
| (1,1839) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 1        | 0.5           |
| (1,1775) | 2:5:B:VAL:HA    | 2:66:B:THR:HG21 | 7        | 0.5           |
| (1,1774) | 2:5:B:VAL:HA    | 2:66:B:THR:HG21 | 7        | 0.5           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1622) | 2:29:B:LYS:HA    | 2:33:B:LYS:HE3  | 3        | 0.5           |
| (1,1535) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG11  | 6        | 0.5           |
| (1,865)  | 1:520:A:ILE:HG12 | 1:562:A:TRP:HE3 | 8        | 0.5           |
| (1,74)   | 1:541:A:ASP:OD1  | 2:74:B:ARG:NH2  | 3        | 0.5           |
| (3,153)  | 2:3:C:ILE:HG21   | 2:67:C:LEU:HG   | 2        | 0.49          |
| (2,3)    | 1:484:A:LYS:O    | 1:488:A:ALA:H   | 4        | 0.49          |
| (1,5900) | 2:66:C:THR:HG22  | 2:68:C:HIS:HB3  | 2        | 0.49          |
| (1,5279) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD22 | 8        | 0.49          |
| (1,4040) | 2:5:C:VAL:HA     | 2:66:C:THR:HG23 | 4        | 0.49          |
| (1,5281) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD22 | 2        | 0.48          |
| (1,4041) | 2:5:C:VAL:HA     | 2:66:C:THR:HG23 | 4        | 0.48          |
| (1,3854) | 2:29:C:LYS:HA    | 2:15:C:LEU:HD13 | 10       | 0.48          |
| (1,3045) | 2:41:B:GLN:H     | 2:71:B:LEU:HD23 | 10       | 0.48          |
| (1,2844) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD23 | 8        | 0.48          |
| (1,5302) | 2:41:C:GLN:HA    | 2:71:C:LEU:HD21 | 7        | 0.47          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG13  | 3        | 0.47          |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD12 | 5        | 0.47          |
| (1,1841) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG23 | 8        | 0.47          |
| (1,1588) | 2:29:B:LYS:HA    | 2:15:B:LEU:HD22 | 3        | 0.47          |
| (1,507)  | 1:575:A:MET:HE1  | 1:575:A:MET:H   | 4        | 0.47          |
| (1,507)  | 1:575:A:MET:HE2  | 1:575:A:MET:H   | 4        | 0.47          |
| (1,507)  | 1:575:A:MET:HE3  | 1:575:A:MET:H   | 4        | 0.47          |
| (1,4040) | 2:5:C:VAL:HA     | 2:66:C:THR:HG21 | 1        | 0.46          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG12  | 1        | 0.46          |
| (1,1840) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22 | 9        | 0.46          |
| (1,1535) | 2:2:B:GLN:HA     | 2:17:B:VAL:HG12 | 3        | 0.46          |
| (1,4041) | 2:5:C:VAL:HA     | 2:66:C:THR:HG21 | 1        | 0.45          |
| (1,4041) | 2:5:C:VAL:HA     | 2:66:C:THR:HG21 | 5        | 0.45          |
| (1,4040) | 2:5:C:VAL:HA     | 2:66:C:THR:HG21 | 5        | 0.45          |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD12 | 2        | 0.45          |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD13 | 9        | 0.45          |
| (1,3758) | 2:1:C:MET:HE3    | 2:56:C:LEU:HD12 | 7        | 0.45          |
| (1,1837) | 2:6:B:LYS:HE3    | 2:66:B:THR:HG22 | 8        | 0.45          |
| (1,1493) | 2:1:B:MET:HE1    | 2:56:B:LEU:HD11 | 5        | 0.45          |
| (1,1390) | 1:599:A:ILE:HD13 | 1:562:A:TRP:HZ3 | 10       | 0.45          |
| (1,5302) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD12 | 9        | 0.44          |
| (1,5280) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD22 | 1        | 0.44          |
| (1,4040) | 2:5:C:VAL:HA     | 2:66:C:THR:HG22 | 8        | 0.44          |
| (1,3802) | 2:2:C:GLN:HE22   | 2:14:C:THR:HG21 | 9        | 0.44          |
| (1,3020) | 2:40:B:GLN:HG2   | 2:71:B:LEU:HD23 | 2        | 0.44          |
| (1,3017) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD21 | 3        | 0.44          |
| (1,3015) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD23 | 7        | 0.44          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1840) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22 | 4        | 0.44          |
| (1,1840) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG21 | 10       | 0.44          |
| (1,1767) | 2:17:B:VAL:HG12  | 2:29:B:LYS:HG3  | 1        | 0.44          |
| (1,1535) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG12  | 4        | 0.44          |
| (1,72)   | 1:591:A:ILE:HD13 | 2:44:B:ILE:HD13 | 8        | 0.44          |
| (1,4203) | 2:12:C:THR:HG22  | 2:13:C:ILE:HA   | 6        | 0.43          |
| (1,4106) | 2:6:C:LYS:HG3    | 2:66:C:THR:HG21 | 3        | 0.43          |
| (1,4072) | 2:11:C:LYS:HG2   | 2:10:C:GLY:HA3  | 5        | 0.43          |
| (1,4041) | 2:5:C:VAL:HA     | 2:66:C:THR:HG22 | 8        | 0.43          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG13  | 4        | 0.43          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG11  | 10       | 0.43          |
| (1,3778) | 2:1:C:MET:HE3    | 2:67:C:LEU:HD12 | 6        | 0.43          |
| (1,3778) | 2:1:C:MET:HE2    | 2:67:C:LEU:HD11 | 10       | 0.43          |
| (1,3759) | 2:1:C:MET:HE3    | 2:56:C:LEU:HD13 | 2        | 0.43          |
| (1,3759) | 2:1:C:MET:HE3    | 2:56:C:LEU:HD11 | 5        | 0.43          |
| (1,3758) | 2:1:C:MET:HE3    | 2:56:C:LEU:HD13 | 10       | 0.43          |
| (1,263)  | 1:516:A:THR:HA   | 1:518:A:LEU:H   | 1        | 0.43          |
| (3,259)  | 2:66:C:THR:HG21  | 2:67:C:LEU:HD23 | 6        | 0.42          |
| (1,5301) | 2:41:C:GLN:HA    | 2:71:C:LEU:HD21 | 7        | 0.42          |
| (1,4339) | 2:15:C:LEU:HD13  | 2:33:C:LYS:HD2  | 6        | 0.42          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG11  | 6        | 0.42          |
| (1,3012) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD22 | 8        | 0.42          |
| (3,24)   | 2:1:B:MET:HE1    | 2:67:B:LEU:HD12 | 7        | 0.41          |
| (1,5302) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD13 | 5        | 0.41          |
| (1,5281) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD23 | 6        | 0.41          |
| (1,5279) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD21 | 9        | 0.41          |
| (1,4339) | 2:15:C:LEU:HD12  | 2:33:C:LYS:HD2  | 5        | 0.41          |
| (1,4072) | 2:11:C:LYS:HG2   | 2:10:C:GLY:HA3  | 7        | 0.41          |
| (1,4033) | 2:17:C:VAL:HG13  | 2:29:C:LYS:HG3  | 3        | 0.41          |
| (1,3036) | 2:41:B:GLN:HA    | 2:69:B:LEU:HD23 | 2        | 0.41          |
| (1,1775) | 2:5:B:VAL:HA     | 2:66:B:THR:HG21 | 10       | 0.41          |
| (1,1774) | 2:5:B:VAL:HA     | 2:66:B:THR:HG21 | 10       | 0.41          |
| (1,1767) | 2:17:B:VAL:HG12  | 2:29:B:LYS:HG3  | 5        | 0.41          |
| (1,1748) | 2:5:B:VAL:HG22   | 2:15:B:LEU:HG   | 5        | 0.41          |
| (2,4)    | 1:484:A:LYS:O    | 1:488:A:ALA:N   | 7        | 0.4           |
| (2,4)    | 1:484:A:LYS:O    | 1:488:A:ALA:N   | 10       | 0.4           |
| (1,5301) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD12 | 9        | 0.4           |
| (1,4322) | 2:15:C:LEU:HD11  | 2:29:C:LYS:HG2  | 7        | 0.4           |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD13  | 3        | 0.4           |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD13  | 10       | 0.4           |
| (1,3050) | 2:42:B:ARG:HA    | 2:69:B:LEU:HD23 | 4        | 0.4           |
| (1,3036) | 2:41:B:GLN:HA    | 2:69:B:LEU:HD12 | 8        | 0.4           |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3012) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD23 | 1        | 0.4           |
| (1,2073) | 2:15:B:LEU:HD22  | 2:33:B:LYS:HD2  | 9        | 0.4           |
| (1,1838) | 2:6:B:LYS:HG2    | 2:66:B:THR:HG23 | 2        | 0.4           |
| (1,1837) | 2:6:B:LYS:HE3    | 2:66:B:THR:HG23 | 7        | 0.4           |
| (1,1836) | 2:6:B:LYS:HD2    | 2:66:B:THR:HG21 | 1        | 0.4           |
| (1,76)   | 1:552:A:GLU:OE2  | 2:42:B:ARG:NH1  | 2        | 0.4           |
| (3,26)   | 2:2:B:GLN:HG3    | 2:3:B:ILE:HA    | 5        | 0.39          |
| (1,5900) | 2:70:C:VAL:HG12  | 2:68:C:HIS:HB3  | 9        | 0.39          |
| (1,5280) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD22 | 2        | 0.39          |
| (1,5186) | 2:36:C:ILE:HG23  | 2:71:C:LEU:HD23 | 4        | 0.39          |
| (1,4205) | 2:12:C:THR:HG21  | 2:13:C:ILE:H    | 4        | 0.39          |
| (1,4040) | 2:5:C:VAL:HA     | 2:66:C:THR:HG22 | 3        | 0.39          |
| (1,3699) | 2:1:C:MET:HE1    | 2:3:C:ILE:HD12  | 8        | 0.39          |
| (1,1840) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22 | 1        | 0.39          |
| (1,1560) | 2:3:B:ILE:HA     | 2:3:B:ILE:HD12  | 5        | 0.39          |
| (1,414)  | 1:547:A:MET:HE1  | 1:548:A:ASP:H   | 6        | 0.39          |
| (1,414)  | 1:547:A:MET:HE2  | 1:548:A:ASP:H   | 6        | 0.39          |
| (1,414)  | 1:547:A:MET:HE3  | 1:548:A:ASP:H   | 6        | 0.39          |
| (1,73)   | 1:591:A:ILE:HG21 | 2:44:B:ILE:HG22 | 8        | 0.39          |
| (1,5311) | 2:41:C:GLN:H     | 2:71:C:LEU:HD22 | 2        | 0.38          |
| (1,4339) | 2:15:C:LEU:HD22  | 2:33:C:LYS:HD2  | 9        | 0.38          |
| (1,4041) | 2:5:C:VAL:HA     | 2:66:C:THR:HG22 | 3        | 0.38          |
| (1,3699) | 2:1:C:MET:HE2    | 2:3:C:ILE:HD12  | 2        | 0.38          |
| (1,2845) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD23 | 8        | 0.38          |
| (1,2073) | 2:15:B:LEU:HD23  | 2:33:B:LYS:HD2  | 3        | 0.38          |
| (1,1588) | 2:29:B:LYS:HA    | 2:15:B:LEU:HD22 | 8        | 0.38          |
| (1,1588) | 2:29:B:LYS:HA    | 2:15:B:LEU:HD13 | 10       | 0.38          |
| (1,1493) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD13 | 4        | 0.38          |
| (1,1493) | 2:1:B:MET:HE3    | 2:56:B:LEU:HD13 | 10       | 0.38          |
| (1,258)  | 1:516:A:THR:H    | 1:518:A:LEU:H   | 1        | 0.38          |
| (1,73)   | 1:591:A:ILE:HG23 | 2:44:B:ILE:HG23 | 1        | 0.38          |
| (3,139)  | 2:66:B:THR:HG21  | 2:67:B:LEU:HD22 | 6        | 0.37          |
| (1,5301) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD13 | 5        | 0.37          |
| (1,3888) | 2:29:C:LYS:HA    | 2:33:C:LYS:HE3  | 5        | 0.37          |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD13  | 1        | 0.37          |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD11  | 5        | 0.37          |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD12  | 8        | 0.37          |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD13  | 9        | 0.37          |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG12  | 5        | 0.37          |
| (1,3035) | 2:41:B:GLN:HA    | 2:69:B:LEU:HD23 | 2        | 0.37          |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD23 | 10       | 0.37          |
| (1,1560) | 2:3:B:ILE:HA     | 2:3:B:ILE:HD13  | 3        | 0.37          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1560) | 2:3:B:ILE:HA    | 2:3:B:ILE:HD11  | 10       | 0.37          |
| (1,1452) | 2:1:B:MET:HE3   | 2:17:B:VAL:HG22 | 3        | 0.37          |
| (1,414)  | 1:547:A:MET:HE1 | 1:548:A:ASP:H   | 5        | 0.37          |
| (1,414)  | 1:547:A:MET:HE2 | 1:548:A:ASP:H   | 5        | 0.37          |
| (1,414)  | 1:547:A:MET:HE3 | 1:548:A:ASP:H   | 5        | 0.37          |
| (3,146)  | 2:2:C:GLN:HG2   | 2:3:C:ILE:HA    | 6        | 0.36          |
| (1,3826) | 2:3:C:ILE:HA    | 2:3:C:ILE:HD12  | 7        | 0.36          |
| (1,3036) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD11 | 9        | 0.36          |
| (1,3035) | 2:41:B:GLN:HA   | 2:69:B:LEU:HD12 | 8        | 0.36          |
| (1,1775) | 2:5:B:VAL:HA    | 2:66:B:THR:HG21 | 8        | 0.36          |
| (1,1774) | 2:5:B:VAL:HA    | 2:66:B:THR:HG21 | 8        | 0.36          |
| (1,1560) | 2:3:B:ILE:HA    | 2:3:B:ILE:HD13  | 6        | 0.36          |
| (1,1560) | 2:3:B:ILE:HA    | 2:3:B:ILE:HD12  | 8        | 0.36          |
| (1,1493) | 2:1:B:MET:HE3   | 2:56:B:LEU:HD13 | 6        | 0.36          |
| (1,1433) | 2:1:B:MET:HE2   | 2:3:B:ILE:HD13  | 2        | 0.36          |
| (1,1433) | 2:1:B:MET:HE2   | 2:3:B:ILE:HD12  | 4        | 0.36          |
| (3,146)  | 2:2:C:GLN:HG2   | 2:3:C:ILE:HA    | 1        | 0.35          |
| (1,5185) | 2:36:C:ILE:HG22 | 2:71:C:LEU:HD22 | 7        | 0.35          |
| (1,4104) | 2:6:C:LYS:HG2   | 2:66:C:THR:HG21 | 4        | 0.35          |
| (1,4072) | 2:11:C:LYS:HG2  | 2:10:C:GLY:HA3  | 2        | 0.35          |
| (1,4041) | 2:5:C:VAL:HA    | 2:66:C:THR:HG23 | 9        | 0.35          |
| (1,4040) | 2:5:C:VAL:HA    | 2:66:C:THR:HG23 | 9        | 0.35          |
| (1,3854) | 2:29:C:LYS:HA   | 2:15:C:LEU:HD22 | 1        | 0.35          |
| (1,3759) | 2:1:C:MET:HE3   | 2:56:C:LEU:HD13 | 9        | 0.35          |
| (1,3014) | 2:40:B:GLN:HB2  | 2:71:B:LEU:HD23 | 7        | 0.35          |
| (1,2073) | 2:15:B:LEU:HD12 | 2:33:B:LYS:HD2  | 1        | 0.35          |
| (1,1560) | 2:3:B:ILE:HA    | 2:3:B:ILE:HD12  | 4        | 0.35          |
| (1,1512) | 2:1:B:MET:HE1   | 2:67:B:LEU:HD11 | 4        | 0.35          |
| (1,1493) | 2:1:B:MET:HE2   | 2:56:B:LEU:HD11 | 9        | 0.35          |
| (1,448)  | 1:554:A:THR:HB  | 1:555:A:ALA:H   | 2        | 0.35          |
| (1,122)  | 1:503:A:ASP:H   | 1:506:A:LEU:H   | 8        | 0.35          |
| (3,146)  | 2:2:C:GLN:HG2   | 2:3:C:ILE:HA    | 8        | 0.34          |
| (3,26)   | 2:2:B:GLN:HG2   | 2:3:B:ILE:HA    | 6        | 0.34          |
| (1,4232) | 2:13:C:ILE:HG21 | 2:15:C:LEU:HD11 | 4        | 0.34          |
| (1,4104) | 2:6:C:LYS:HG3   | 2:66:C:THR:HG21 | 2        | 0.34          |
| (1,4041) | 2:5:C:VAL:HA    | 2:66:C:THR:HG21 | 7        | 0.34          |
| (1,4040) | 2:5:C:VAL:HA    | 2:66:C:THR:HG21 | 7        | 0.34          |
| (1,3758) | 2:1:C:MET:HE1   | 2:56:C:LEU:HD12 | 3        | 0.34          |
| (1,3699) | 2:1:C:MET:HE3   | 2:3:C:ILE:HD12  | 7        | 0.34          |
| (1,3699) | 2:1:C:MET:HE2   | 2:3:C:ILE:HD13  | 9        | 0.34          |
| (1,1588) | 2:29:B:LYS:HA   | 2:15:B:LEU:HD12 | 5        | 0.34          |
| (1,1493) | 2:1:B:MET:HE1   | 2:56:B:LEU:HD13 | 8        | 0.34          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (3,224)  | 2:36:C:ILE:HA    | 2:71:C:LEU:HD22 | 3        | 0.33          |
| (1,5185) | 2:36:C:ILE:HG22  | 2:71:C:LEU:HD22 | 3        | 0.33          |
| (1,4318) | 2:15:C:LEU:HD12  | 2:29:C:LYS:HA   | 8        | 0.33          |
| (1,4149) | 2:7:C:THR:HA     | 2:69:C:LEU:HD22 | 4        | 0.33          |
| (1,3802) | 2:2:C:GLN:HE22   | 2:14:C:THR:HG22 | 3        | 0.33          |
| (1,3802) | 2:2:C:GLN:HE22   | 2:14:C:THR:HG22 | 8        | 0.33          |
| (1,3778) | 2:1:C:MET:HE1    | 2:67:C:LEU:HD11 | 4        | 0.33          |
| (1,3759) | 2:1:C:MET:HE2    | 2:56:C:LEU:HD12 | 4        | 0.33          |
| (1,3759) | 2:1:C:MET:HE1    | 2:56:C:LEU:HD11 | 6        | 0.33          |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD23 | 7        | 0.33          |
| (1,1839) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG21 | 7        | 0.33          |
| (1,1622) | 2:29:B:LYS:HA    | 2:33:B:LYS:HE3  | 10       | 0.33          |
| (1,1588) | 2:29:B:LYS:HA    | 2:15:B:LEU:HD13 | 7        | 0.33          |
| (3,259)  | 2:66:C:THR:HG23  | 2:67:C:LEU:HD21 | 8        | 0.32          |
| (3,146)  | 2:2:C:GLN:HG2    | 2:3:C:ILE:HA    | 3        | 0.32          |
| (1,5900) | 2:70:C:VAL:HG13  | 2:68:C:HIS:HB3  | 8        | 0.32          |
| (1,5302) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD13 | 4        | 0.32          |
| (1,5302) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD11 | 6        | 0.32          |
| (1,5280) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD23 | 6        | 0.32          |
| (1,4322) | 2:15:C:LEU:HD12  | 2:29:C:LYS:HG3  | 8        | 0.32          |
| (1,4102) | 2:6:C:LYS:HD2    | 2:66:C:THR:HG23 | 3        | 0.32          |
| (1,4040) | 2:5:C:VAL:HA     | 2:66:C:THR:HG21 | 6        | 0.32          |
| (1,3888) | 2:29:C:LYS:HA    | 2:33:C:LYS:HE2  | 1        | 0.32          |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD11  | 6        | 0.32          |
| (1,3036) | 2:41:B:GLN:HA    | 2:69:B:LEU:HD13 | 1        | 0.32          |
| (1,3035) | 2:41:B:GLN:HA    | 2:69:B:LEU:HD11 | 9        | 0.32          |
| (1,1882) | 2:7:B:THR:HA     | 2:69:B:LEU:HD22 | 9        | 0.32          |
| (1,1135) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HB2 | 9        | 0.32          |
| (1,1135) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HB3 | 9        | 0.32          |
| (1,1135) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HB2 | 9        | 0.32          |
| (1,1135) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HB3 | 9        | 0.32          |
| (1,1135) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HB2 | 9        | 0.32          |
| (1,1135) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HB3 | 9        | 0.32          |
| (3,26)   | 2:2:B:GLN:HG2    | 2:3:B:ILE:HA    | 10       | 0.31          |
| (2,3)    | 1:484:A:LYS:O    | 1:488:A:ALA:H   | 10       | 0.31          |
| (1,5311) | 2:41:C:GLN:H     | 2:69:C:LEU:HD13 | 3        | 0.31          |
| (1,5302) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD11 | 10       | 0.31          |
| (1,4203) | 2:12:C:THR:HG22  | 2:13:C:ILE:HA   | 7        | 0.31          |
| (1,4041) | 2:5:C:VAL:HA     | 2:66:C:THR:HG21 | 6        | 0.31          |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD12  | 4        | 0.31          |
| (1,3719) | 2:1:C:MET:HG2    | 2:17:C:VAL:HG21 | 1        | 0.31          |
| (1,3719) | 2:1:C:MET:HG2    | 2:17:C:VAL:HG22 | 1        | 0.31          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3719) | 2:1:C:MET:HG2    | 2:17:C:VAL:HG23 | 1        | 0.31          |
| (1,3719) | 2:1:C:MET:HG3    | 2:17:C:VAL:HG21 | 1        | 0.31          |
| (1,3719) | 2:1:C:MET:HG3    | 2:17:C:VAL:HG22 | 1        | 0.31          |
| (1,3719) | 2:1:C:MET:HG3    | 2:17:C:VAL:HG23 | 1        | 0.31          |
| (1,3019) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD21 | 3        | 0.31          |
| (1,1767) | 2:17:B:VAL:HG12  | 2:29:B:LYS:HG3  | 6        | 0.31          |
| (1,1560) | 2:3:B:ILE:HA     | 2:3:B:ILE:HD11  | 1        | 0.31          |
| (1,1560) | 2:3:B:ILE:HA     | 2:3:B:ILE:HD13  | 7        | 0.31          |
| (1,1560) | 2:3:B:ILE:HA     | 2:3:B:ILE:HD11  | 9        | 0.31          |
| (1,1535) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG13  | 1        | 0.31          |
| (1,1494) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD12 | 1        | 0.31          |
| (1,414)  | 1:547:A:MET:HE1  | 1:548:A:ASP:H   | 10       | 0.31          |
| (1,414)  | 1:547:A:MET:HE2  | 1:548:A:ASP:H   | 10       | 0.31          |
| (1,414)  | 1:547:A:MET:HE3  | 1:548:A:ASP:H   | 10       | 0.31          |
| (2,3)    | 1:484:A:LYS:O    | 1:488:A:ALA:H   | 7        | 0.3           |
| (1,5185) | 2:36:C:ILE:HG22  | 2:71:C:LEU:HD22 | 1        | 0.3           |
| (1,4205) | 2:12:C:THR:HG21  | 2:13:C:ILE:H    | 6        | 0.3           |
| (1,4203) | 2:12:C:THR:HG22  | 2:13:C:ILE:HA   | 4        | 0.3           |
| (1,4123) | 2:7:C:THR:HB     | 2:9:C:THR:H     | 5        | 0.3           |
| (1,3826) | 2:3:C:ILE:HA     | 2:3:C:ILE:HD13  | 2        | 0.3           |
| (1,3801) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG11  | 2        | 0.3           |
| (1,3699) | 2:1:C:MET:HE2    | 2:3:C:ILE:HD11  | 5        | 0.3           |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD21 | 3        | 0.3           |
| (1,1750) | 2:5:B:VAL:HG22   | 2:15:B:LEU:HG   | 9        | 0.3           |
| (1,1163) | 1:563:A:VAL:HG22 | 1:562:A:TRP:HZ2 | 7        | 0.3           |
| (1,507)  | 1:575:A:MET:HE1  | 1:575:A:MET:H   | 2        | 0.3           |
| (1,507)  | 1:575:A:MET:HE2  | 1:575:A:MET:H   | 2        | 0.3           |
| (1,507)  | 1:575:A:MET:HE3  | 1:575:A:MET:H   | 2        | 0.3           |
| (1,460)  | 1:556:A:ILE:H    | 1:557:A:GLU:H   | 1        | 0.3           |
| (1,5285) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD23 | 4        | 0.29          |
| (1,5278) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD23 | 6        | 0.29          |
| (1,3888) | 2:29:C:LYS:HA    | 2:33:C:LYS:HE2  | 7        | 0.29          |
| (1,3854) | 2:29:C:LYS:HA    | 2:15:C:LEU:HD12 | 9        | 0.29          |
| (1,459)  | 1:555:A:ALA:HB1  | 1:558:A:LEU:H   | 3        | 0.29          |
| (1,459)  | 1:555:A:ALA:HB2  | 1:558:A:LEU:H   | 3        | 0.29          |
| (1,459)  | 1:555:A:ALA:HB3  | 1:558:A:LEU:H   | 3        | 0.29          |
| (1,5301) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD13 | 4        | 0.28          |
| (1,5301) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD11 | 6        | 0.28          |
| (1,3854) | 2:29:C:LYS:HA    | 2:15:C:LEU:HD12 | 3        | 0.28          |
| (1,3045) | 2:41:B:GLN:H     | 2:71:B:LEU:HD21 | 5        | 0.28          |
| (1,3036) | 2:41:B:GLN:HA    | 2:71:B:LEU:HD22 | 10       | 0.28          |
| (1,3035) | 2:41:B:GLN:HA    | 2:69:B:LEU:HD13 | 1        | 0.28          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1996) | 2:13:B:ILE:HG12 | 2:34:B:GLU:HG3  | 9        | 0.28          |
| (1,1766) | 2:17:B:VAL:HG13 | 2:29:B:LYS:HG3  | 3        | 0.28          |
| (1,1560) | 2:3:B:ILE:HA    | 2:3:B:ILE:HD11  | 2        | 0.28          |
| (1,1453) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG21 | 1        | 0.28          |
| (1,1453) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG22 | 1        | 0.28          |
| (1,1453) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG23 | 1        | 0.28          |
| (1,1453) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG21 | 1        | 0.28          |
| (1,1453) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG22 | 1        | 0.28          |
| (1,1453) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG23 | 1        | 0.28          |
| (1,1452) | 2:1:B:MET:HE2   | 2:17:B:VAL:HG23 | 10       | 0.28          |
| (1,1433) | 2:1:B:MET:HE3   | 2:3:B:ILE:HD12  | 8        | 0.28          |
| (3,24)   | 2:1:B:MET:HE2   | 2:67:B:LEU:HD13 | 6        | 0.27          |
| (1,5301) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD11 | 10       | 0.27          |
| (1,4160) | 2:7:C:THR:HG23  | 2:69:C:LEU:HD21 | 8        | 0.27          |
| (1,4040) | 2:5:C:VAL:HA    | 2:66:C:THR:HG22 | 2        | 0.27          |
| (1,4033) | 2:17:C:VAL:HG13 | 2:29:C:LYS:HG3  | 8        | 0.27          |
| (1,3699) | 2:1:C:MET:HE3   | 2:3:C:ILE:HD11  | 6        | 0.27          |
| (1,3045) | 2:41:B:GLN:H    | 2:69:B:LEU:HD12 | 3        | 0.27          |
| (1,2919) | 2:36:B:ILE:HG22 | 2:71:B:LEU:HD13 | 9        | 0.27          |
| (1,1749) | 2:5:B:VAL:HG23  | 2:13:B:ILE:HG13 | 10       | 0.27          |
| (1,1492) | 2:1:B:MET:HE1   | 2:56:B:LEU:HD11 | 5        | 0.27          |
| (1,122)  | 1:503:A:ASP:H   | 1:506:A:LEU:H   | 2        | 0.27          |
| (2,4)    | 1:484:A:LYS:O   | 1:488:A:ALA:N   | 2        | 0.26          |
| (1,5302) | 2:41:C:GLN:HA   | 2:69:C:LEU:HD11 | 8        | 0.26          |
| (1,4339) | 2:15:C:LEU:HD13 | 2:33:C:LYS:HD2  | 4        | 0.26          |
| (1,4155) | 2:7:C:THR:HB    | 2:69:C:LEU:HD21 | 8        | 0.26          |
| (1,4041) | 2:5:C:VAL:HA    | 2:66:C:THR:HG22 | 2        | 0.26          |
| (1,3758) | 2:1:C:MET:HE3   | 2:56:C:LEU:HD13 | 2        | 0.26          |
| (1,3714) | 2:1:C:MET:HE3   | 2:17:C:VAL:HB   | 2        | 0.26          |
| (1,3015) | 2:40:B:GLN:HB2  | 2:71:B:LEU:HD23 | 10       | 0.26          |
| (1,2924) | 2:36:B:ILE:HG23 | 2:71:B:LEU:HD11 | 8        | 0.26          |
| (1,1622) | 2:29:B:LYS:HA   | 2:33:B:LYS:HE2  | 5        | 0.26          |
| (1,1493) | 2:1:B:MET:HE1   | 2:56:B:LEU:HD13 | 7        | 0.26          |
| (1,1452) | 2:1:B:MET:HE3   | 2:17:B:VAL:HG22 | 5        | 0.26          |
| (3,33)   | 2:3:B:ILE:HG22  | 2:67:B:LEU:HG   | 9        | 0.25          |
| (3,26)   | 2:2:B:GLN:HG2   | 2:3:B:ILE:HA    | 3        | 0.25          |
| (3,26)   | 2:2:B:GLN:HG2   | 2:3:B:ILE:HA    | 9        | 0.25          |
| (1,4206) | 2:14:C:THR:HG21 | 2:14:C:THR:H    | 3        | 0.25          |
| (1,3888) | 2:29:C:LYS:HA   | 2:33:C:LYS:HE2  | 9        | 0.25          |
| (1,3761) | 2:1:C:MET:HE1   | 2:56:C:LEU:HD12 | 1        | 0.25          |
| (1,3758) | 2:1:C:MET:HE3   | 2:56:C:LEU:HD11 | 5        | 0.25          |
| (1,3017) | 2:40:B:GLN:HB3  | 2:71:B:LEU:HD22 | 8        | 0.25          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,2924) | 2:36:B:ILE:HG23  | 2:71:B:LEU:HD13 | 1        | 0.25          |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD21 | 1        | 0.25          |
| (1,1836) | 2:6:B:LYS:HD2    | 2:66:B:THR:HG23 | 7        | 0.25          |
| (1,1559) | 2:68:B:HIS:HA    | 2:66:B:THR:HG22 | 10       | 0.25          |
| (1,1509) | 2:1:B:MET:HG2    | 2:63:B:LYS:HA   | 1        | 0.25          |
| (1,1509) | 2:1:B:MET:HG3    | 2:63:B:LYS:HA   | 1        | 0.25          |
| (1,1448) | 2:1:B:MET:HE3    | 2:17:B:VAL:HB   | 3        | 0.25          |
| (1,3888) | 2:29:C:LYS:HA    | 2:33:C:LYS:HE3  | 6        | 0.24          |
| (1,3718) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG22 | 2        | 0.24          |
| (1,3718) | 2:1:C:MET:HE3    | 2:17:C:VAL:HG22 | 5        | 0.24          |
| (1,3035) | 2:41:B:GLN:HA    | 2:71:B:LEU:HD22 | 10       | 0.24          |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD22 | 5        | 0.24          |
| (1,1727) | 2:5:B:VAL:HG12   | 2:7:B:THR:HA    | 2        | 0.24          |
| (1,1622) | 2:29:B:LYS:HA    | 2:33:B:LYS:HE2  | 4        | 0.24          |
| (1,1588) | 2:29:B:LYS:HA    | 2:15:B:LEU:HD21 | 1        | 0.24          |
| (1,1559) | 2:68:B:HIS:HA    | 2:66:B:THR:HG23 | 9        | 0.24          |
| (1,1390) | 1:599:A:ILE:HD13 | 1:562:A:TRP:HD1 | 9        | 0.24          |
| (1,5281) | 2:40:C:GLN:HB2   | 2:71:C:LEU:HD23 | 5        | 0.23          |
| (1,4203) | 2:12:C:THR:HG22  | 2:13:C:ILE:HA   | 1        | 0.23          |
| (1,4203) | 2:12:C:THR:HG23  | 2:13:C:ILE:HA   | 5        | 0.23          |
| (1,4203) | 2:12:C:THR:HG21  | 2:13:C:ILE:HA   | 9        | 0.23          |
| (1,4015) | 2:5:C:VAL:HG23   | 2:13:C:ILE:HG13 | 8        | 0.23          |
| (1,3017) | 2:40:B:GLN:HB3   | 2:71:B:LEU:HD23 | 1        | 0.23          |
| (1,2924) | 2:36:B:ILE:HG21  | 2:71:B:LEU:HD13 | 3        | 0.23          |
| (1,2073) | 2:15:B:LEU:HD21  | 2:33:B:LYS:HD2  | 8        | 0.23          |
| (1,1775) | 2:5:B:VAL:HA     | 2:66:B:THR:HG23 | 2        | 0.23          |
| (1,1774) | 2:5:B:VAL:HA     | 2:66:B:THR:HG23 | 2        | 0.23          |
| (1,1774) | 2:5:B:VAL:HA     | 2:66:B:THR:HG21 | 5        | 0.23          |
| (3,52)   | 2:34:B:GLU:HG3   | 2:30:B:ILE:HD13 | 4        | 0.22          |
| (3,26)   | 2:2:B:GLN:HG2    | 2:3:B:ILE:HA    | 1        | 0.22          |
| (1,5308) | 2:41:C:GLN:HG2   | 2:69:C:LEU:HD11 | 7        | 0.22          |
| (1,5301) | 2:41:C:GLN:HA    | 2:69:C:LEU:HD11 | 8        | 0.22          |
| (1,4155) | 2:7:C:THR:HB     | 2:69:C:LEU:HD23 | 2        | 0.22          |
| (1,4033) | 2:17:C:VAL:HG12  | 2:29:C:LYS:HG3  | 7        | 0.22          |
| (1,3740) | 2:28:C:ALA:HB2   | 2:25:C:ASN:HA   | 9        | 0.22          |
| (1,2056) | 2:15:B:LEU:HD12  | 2:29:B:LYS:HG2  | 5        | 0.22          |
| (1,1840) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG21 | 7        | 0.22          |
| (1,1775) | 2:5:B:VAL:HA     | 2:66:B:THR:HG21 | 5        | 0.22          |
| (1,1749) | 2:5:B:VAL:HG22   | 2:13:B:ILE:HG13 | 2        | 0.22          |
| (1,1622) | 2:29:B:LYS:HA    | 2:33:B:LYS:HE3  | 9        | 0.22          |
| (1,1452) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG22 | 2        | 0.22          |
| (1,1448) | 2:1:B:MET:HE2    | 2:17:B:VAL:HB   | 2        | 0.22          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,1448) | 2:1:B:MET:HE3    | 2:17:B:VAL:HB   | 10       | 0.22          |
| (1,5305) | 2:41:C:GLN:HB3   | 2:69:C:LEU:HD12 | 1        | 0.21          |
| (1,4160) | 2:7:C:THR:HG23   | 2:69:C:LEU:HD23 | 2        | 0.21          |
| (1,3714) | 2:1:C:MET:HE3    | 2:17:C:VAL:HB   | 5        | 0.21          |
| (1,2056) | 2:15:B:LEU:HD13  | 2:29:B:LYS:HG2  | 7        | 0.21          |
| (1,1838) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG23 | 6        | 0.21          |
| (1,1749) | 2:5:B:VAL:HG22   | 2:13:B:ILE:HG13 | 5        | 0.21          |
| (1,1559) | 2:68:B:HIS:HA    | 2:66:B:THR:HG22 | 7        | 0.21          |
| (1,1535) | 2:68:B:HIS:HA    | 2:5:B:VAL:HG11  | 10       | 0.21          |
| (1,122)  | 1:503:A:ASP:H    | 1:506:A:LEU:H   | 9        | 0.21          |
| (3,146)  | 2:2:C:GLN:HG2    | 2:3:C:ILE:HA    | 5        | 0.2           |
| (1,5900) | 2:70:C:VAL:HG13  | 2:68:C:HIS:HB3  | 10       | 0.2           |
| (1,5302) | 2:41:C:GLN:HA    | 2:71:C:LEU:HD22 | 2        | 0.2           |
| (1,5278) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD23 | 5        | 0.2           |
| (1,4322) | 2:15:C:LEU:HD12  | 2:29:C:LYS:HG3  | 1        | 0.2           |
| (1,4206) | 2:14:C:THR:HG21  | 2:14:C:THR:H    | 2        | 0.2           |
| (1,4160) | 2:7:C:THR:HG22   | 2:69:C:LEU:HD21 | 10       | 0.2           |
| (1,3740) | 2:28:C:ALA:HB2   | 2:25:C:ASN:HA   | 4        | 0.2           |
| (1,3718) | 2:1:C:MET:HE1    | 2:17:C:VAL:HG23 | 8        | 0.2           |
| (1,1836) | 2:6:B:LYS:HD2    | 2:66:B:THR:HG21 | 4        | 0.2           |
| (1,1511) | 2:1:B:MET:HG3    | 2:63:B:LYS:HA   | 7        | 0.2           |
| (1,1492) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD13 | 4        | 0.2           |
| (1,1492) | 2:1:B:MET:HE3    | 2:56:B:LEU:HD13 | 10       | 0.2           |
| (1,1452) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG21 | 6        | 0.2           |
| (1,1136) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HG2 | 9        | 0.2           |
| (1,1136) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HG3 | 9        | 0.2           |
| (1,1136) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HG2 | 9        | 0.2           |
| (1,1136) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HG3 | 9        | 0.2           |
| (1,1136) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HG2 | 9        | 0.2           |
| (1,1136) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HG3 | 9        | 0.2           |
| (1,122)  | 1:503:A:ASP:H    | 1:506:A:LEU:H   | 4        | 0.2           |
| (1,5185) | 2:36:C:ILE:HG21  | 2:71:C:LEU:HD23 | 5        | 0.19          |
| (1,3705) | 2:1:C:MET:HG2    | 2:3:C:ILE:HG21  | 1        | 0.19          |
| (1,3705) | 2:1:C:MET:HG2    | 2:3:C:ILE:HG22  | 1        | 0.19          |
| (1,3705) | 2:1:C:MET:HG2    | 2:3:C:ILE:HG23  | 1        | 0.19          |
| (1,3705) | 2:1:C:MET:HG3    | 2:3:C:ILE:HG21  | 1        | 0.19          |
| (1,3705) | 2:1:C:MET:HG3    | 2:3:C:ILE:HG22  | 1        | 0.19          |
| (1,3705) | 2:1:C:MET:HG3    | 2:3:C:ILE:HG23  | 1        | 0.19          |
| (1,3644) | 2:67:B:LEU:HB3   | 2:68:B:HIS:H    | 1        | 0.19          |
| (1,2052) | 2:15:B:LEU:HD13  | 2:29:B:LYS:HA   | 2        | 0.19          |
| (1,1534) | 2:2:B:GLN:HA     | 2:17:B:VAL:HG12 | 2        | 0.19          |
| (1,1492) | 2:1:B:MET:HE3    | 2:56:B:LEU:HD13 | 6        | 0.19          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1488) | 2:1:B:MET:HE2   | 2:56:B:LEU:HB3  | 1        | 0.19          |
| (1,1452) | 2:1:B:MET:HE2   | 2:17:B:VAL:HG22 | 9        | 0.19          |
| (1,448)  | 1:554:A:THR:HB  | 1:555:A:ALA:H   | 7        | 0.19          |
| (3,26)   | 2:2:B:GLN:HG2   | 2:3:B:ILE:HA    | 8        | 0.18          |
| (1,5910) | 2:67:C:LEU:HB3  | 2:68:C:HIS:H    | 2        | 0.18          |
| (1,5278) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD22 | 8        | 0.18          |
| (1,4318) | 2:15:C:LEU:HD11 | 2:29:C:LYS:HA   | 7        | 0.18          |
| (1,4285) | 2:15:C:LEU:HA   | 2:15:C:LEU:HD11 | 2        | 0.18          |
| (1,3740) | 2:28:C:ALA:HB3  | 2:25:C:ASN:HA   | 3        | 0.18          |
| (1,3740) | 2:28:C:ALA:HB2  | 2:25:C:ASN:HA   | 5        | 0.18          |
| (1,3721) | 2:1:C:MET:HG2   | 2:17:C:VAL:HG21 | 1        | 0.18          |
| (1,3721) | 2:1:C:MET:HG2   | 2:17:C:VAL:HG22 | 1        | 0.18          |
| (1,3721) | 2:1:C:MET:HG2   | 2:17:C:VAL:HG23 | 1        | 0.18          |
| (1,3721) | 2:1:C:MET:HG3   | 2:17:C:VAL:HG21 | 1        | 0.18          |
| (1,3721) | 2:1:C:MET:HG3   | 2:17:C:VAL:HG22 | 1        | 0.18          |
| (1,3721) | 2:1:C:MET:HG3   | 2:17:C:VAL:HG23 | 1        | 0.18          |
| (1,3718) | 2:1:C:MET:HE3   | 2:17:C:VAL:HG21 | 10       | 0.18          |
| (1,1838) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 3        | 0.18          |
| (1,1511) | 2:1:B:MET:HG3   | 2:63:B:LYS:HA   | 9        | 0.18          |
| (1,1511) | 2:1:B:MET:HG3   | 2:63:B:LYS:HA   | 10       | 0.18          |
| (1,1448) | 2:1:B:MET:HE2   | 2:17:B:VAL:HB   | 4        | 0.18          |
| (1,5010) | 2:30:C:ILE:HG22 | 2:69:C:LEU:HD23 | 1        | 0.17          |
| (1,4339) | 2:15:C:LEU:HD23 | 2:33:C:LYS:HD2  | 1        | 0.17          |
| (1,4206) | 2:14:C:THR:HG21 | 2:14:C:THR:H    | 1        | 0.17          |
| (1,4206) | 2:14:C:THR:HG21 | 2:14:C:THR:H    | 8        | 0.17          |
| (1,4206) | 2:14:C:THR:HG23 | 2:14:C:THR:H    | 9        | 0.17          |
| (1,4155) | 2:7:C:THR:HB    | 2:69:C:LEU:HD23 | 5        | 0.17          |
| (1,3766) | 2:1:C:MET:HE1   | 2:62:C:GLN:HA   | 1        | 0.17          |
| (1,3766) | 2:1:C:MET:HE2   | 2:62:C:GLN:HA   | 1        | 0.17          |
| (1,3766) | 2:1:C:MET:HE3   | 2:62:C:GLN:HA   | 1        | 0.17          |
| (1,3758) | 2:1:C:MET:HE3   | 2:56:C:LEU:HD13 | 9        | 0.17          |
| (1,3714) | 2:1:C:MET:HE1   | 2:17:C:VAL:HB   | 8        | 0.17          |
| (1,3043) | 2:41:B:GLN:HG2  | 2:69:B:LEU:HD13 | 2        | 0.17          |
| (1,3014) | 2:40:B:GLN:HB2  | 2:71:B:LEU:HD23 | 10       | 0.17          |
| (1,2068) | 2:36:B:ILE:HG13 | 2:30:B:ILE:HG21 | 4        | 0.17          |
| (1,2047) | 2:15:B:LEU:HD13 | 2:26:B:VAL:HA   | 10       | 0.17          |
| (1,1997) | 2:13:B:ILE:HG12 | 2:34:B:GLU:HG3  | 9        | 0.17          |
| (1,1940) | 2:14:B:THR:HG22 | 2:14:B:THR:H    | 10       | 0.17          |
| (1,1534) | 2:68:B:HIS:HA   | 2:5:B:VAL:HG11  | 8        | 0.17          |
| (1,1500) | 2:1:B:MET:HE1   | 2:62:B:GLN:HA   | 1        | 0.17          |
| (1,1500) | 2:1:B:MET:HE2   | 2:62:B:GLN:HA   | 1        | 0.17          |
| (1,1500) | 2:1:B:MET:HE3   | 2:62:B:GLN:HA   | 1        | 0.17          |

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| Key      | Atom-1           | Atom-2           | Model ID | Violation (Å) |
|----------|------------------|------------------|----------|---------------|
| (1,1492) | 2:1:B:MET:HE2    | 2:56:B:LEU:HD11  | 9        | 0.17          |
| (1,1474) | 2:28:B:ALA:HB3   | 2:25:B:ASN:HA    | 7        | 0.17          |
| (1,1448) | 2:1:B:MET:HE1    | 2:17:B:VAL:HB    | 7        | 0.17          |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD11 | 3        | 0.17          |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD12 | 3        | 0.17          |
| (1,1120) | 1:554:A:THR:HB   | 1:556:A:ILE:HD13 | 3        | 0.17          |
| (1,486)  | 1:558:A:LEU:HD21 | 1:558:A:LEU:H    | 3        | 0.17          |
| (1,486)  | 1:558:A:LEU:HD22 | 1:558:A:LEU:H    | 3        | 0.17          |
| (1,486)  | 1:558:A:LEU:HD23 | 1:558:A:LEU:H    | 3        | 0.17          |
| (1,407)  | 1:547:A:MET:HE1  | 1:547:A:MET:H    | 7        | 0.17          |
| (1,407)  | 1:547:A:MET:HE2  | 1:547:A:MET:H    | 7        | 0.17          |
| (1,407)  | 1:547:A:MET:HE3  | 1:547:A:MET:H    | 7        | 0.17          |
| (1,5301) | 2:41:C:GLN:HA    | 2:71:C:LEU:HD22  | 2        | 0.16          |
| (1,4155) | 2:7:C:THR:HB     | 2:69:C:LEU:HD22  | 4        | 0.16          |
| (1,3800) | 2:68:C:HIS:HA    | 2:5:C:VAL:HG11   | 9        | 0.16          |
| (1,3718) | 2:1:C:MET:HE2    | 2:17:C:VAL:HG21  | 4        | 0.16          |
| (1,3714) | 2:1:C:MET:HE2    | 2:17:C:VAL:HB    | 4        | 0.16          |
| (1,3714) | 2:1:C:MET:HE3    | 2:17:C:VAL:HB    | 10       | 0.16          |
| (1,3699) | 2:1:C:MET:HE1    | 2:3:C:ILE:HD12   | 4        | 0.16          |
| (1,3041) | 2:41:B:GLN:HG2   | 2:69:B:LEU:HD13  | 2        | 0.16          |
| (1,3019) | 2:40:B:GLN:HB2   | 2:71:B:LEU:HD11  | 9        | 0.16          |
| (1,1941) | 2:14:B:THR:HG23  | 2:15:B:LEU:H     | 1        | 0.16          |
| (1,1940) | 2:14:B:THR:HG22  | 2:14:B:THR:H     | 5        | 0.16          |
| (1,1839) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG23  | 8        | 0.16          |
| (1,1782) | 2:5:B:VAL:HG11   | 2:69:B:LEU:HB3   | 10       | 0.16          |
| (1,1675) | 2:4:B:PHE:HA     | 2:14:B:THR:HG23  | 1        | 0.16          |
| (1,1511) | 2:1:B:MET:HG2    | 2:63:B:LYS:HA    | 3        | 0.16          |
| (1,1492) | 2:1:B:MET:HE1    | 2:56:B:LEU:HD13  | 8        | 0.16          |
| (1,1452) | 2:1:B:MET:HE2    | 2:17:B:VAL:HG21  | 4        | 0.16          |
| (1,1452) | 2:1:B:MET:HE1    | 2:17:B:VAL:HG21  | 7        | 0.16          |
| (1,1451) | 2:1:B:MET:HE3    | 2:17:B:VAL:HG22  | 3        | 0.16          |
| (1,250)  | 1:515:A:SER:H    | 1:517:A:ASP:H    | 10       | 0.16          |
| (1,5279) | 2:40:C:GLN:HB3   | 2:71:C:LEU:HD22  | 3        | 0.15          |
| (1,4869) | 2:27:C:LYS:HB3   | 2:38:C:PRO:HG3   | 2        | 0.15          |
| (1,4203) | 2:12:C:THR:HG22  | 2:13:C:ILE:HA    | 8        | 0.15          |
| (1,4125) | 2:7:C:THR:HG21   | 2:11:C:LYS:HB2   | 9        | 0.15          |
| (1,4125) | 2:7:C:THR:HG21   | 2:11:C:LYS:HB3   | 9        | 0.15          |
| (1,4125) | 2:7:C:THR:HG22   | 2:11:C:LYS:HB2   | 9        | 0.15          |
| (1,4125) | 2:7:C:THR:HG22   | 2:11:C:LYS:HB3   | 9        | 0.15          |
| (1,4125) | 2:7:C:THR:HG23   | 2:11:C:LYS:HB2   | 9        | 0.15          |
| (1,4125) | 2:7:C:THR:HG23   | 2:11:C:LYS:HB3   | 9        | 0.15          |
| (1,3777) | 2:1:C:MET:HG3    | 2:63:C:LYS:HA    | 3        | 0.15          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,3758) | 2:1:C:MET:HE2   | 2:56:C:LEU:HD12 | 4        | 0.15          |
| (1,3758) | 2:1:C:MET:HE1   | 2:56:C:LEU:HD11 | 6        | 0.15          |
| (1,3718) | 2:1:C:MET:HE3   | 2:17:C:VAL:HG22 | 9        | 0.15          |
| (1,3644) | 2:67:B:LEU:HB3  | 2:68:B:HIS:H    | 2        | 0.15          |
| (1,3644) | 2:67:B:LEU:HB3  | 2:68:B:HIS:H    | 5        | 0.15          |
| (1,3016) | 2:40:B:GLN:HB3  | 2:71:B:LEU:HD21 | 3        | 0.15          |
| (1,2056) | 2:15:B:LEU:HD13 | 2:29:B:LYS:HG2  | 10       | 0.15          |
| (1,1940) | 2:14:B:THR:HG21 | 2:14:B:THR:H    | 4        | 0.15          |
| (1,1782) | 2:5:B:VAL:HG13  | 2:69:B:LEU:HB3  | 5        | 0.15          |
| (1,1775) | 2:5:B:VAL:HA    | 2:66:B:THR:HG23 | 3        | 0.15          |
| (1,1774) | 2:5:B:VAL:HA    | 2:66:B:THR:HG23 | 3        | 0.15          |
| (1,1489) | 2:1:B:MET:HE2   | 2:56:B:LEU:HB3  | 1        | 0.15          |
| (1,1474) | 2:28:B:ALA:HB1  | 2:25:B:ASN:HA   | 9        | 0.15          |
| (1,1455) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG21 | 1        | 0.15          |
| (1,1455) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG22 | 1        | 0.15          |
| (1,1455) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG23 | 1        | 0.15          |
| (1,1455) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG21 | 1        | 0.15          |
| (1,1455) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG22 | 1        | 0.15          |
| (1,1455) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG23 | 1        | 0.15          |
| (1,1448) | 2:1:B:MET:HE1   | 2:17:B:VAL:HB   | 5        | 0.15          |
| (1,1439) | 2:1:B:MET:HG2   | 2:3:B:ILE:HG21  | 1        | 0.15          |
| (1,1439) | 2:1:B:MET:HG2   | 2:3:B:ILE:HG22  | 1        | 0.15          |
| (1,1439) | 2:1:B:MET:HG2   | 2:3:B:ILE:HG23  | 1        | 0.15          |
| (1,1439) | 2:1:B:MET:HG3   | 2:3:B:ILE:HG21  | 1        | 0.15          |
| (1,1439) | 2:1:B:MET:HG3   | 2:3:B:ILE:HG22  | 1        | 0.15          |
| (1,1439) | 2:1:B:MET:HG3   | 2:3:B:ILE:HG23  | 1        | 0.15          |
| (1,414)  | 1:547:A:MET:HE1 | 1:548:A:ASP:H   | 4        | 0.15          |
| (1,414)  | 1:547:A:MET:HE2 | 1:548:A:ASP:H   | 4        | 0.15          |
| (1,414)  | 1:547:A:MET:HE3 | 1:548:A:ASP:H   | 4        | 0.15          |
| (1,5280) | 2:40:C:GLN:HB2  | 2:71:C:LEU:HD23 | 5        | 0.14          |
| (1,4313) | 2:43:C:LEU:HD12 | 2:26:C:VAL:HA   | 6        | 0.14          |
| (1,4206) | 2:14:C:THR:HG21 | 2:14:C:THR:H    | 4        | 0.14          |
| (1,4072) | 2:11:C:LYS:HG2  | 2:10:C:GLY:HA3  | 8        | 0.14          |
| (1,3994) | 2:5:C:VAL:HG12  | 2:7:C:THR:HG22  | 8        | 0.14          |
| (1,3740) | 2:28:C:ALA:HB3  | 2:25:C:ASN:HA   | 1        | 0.14          |
| (1,3722) | 2:1:C:MET:HG2   | 2:17:C:VAL:HG21 | 1        | 0.14          |
| (1,3722) | 2:1:C:MET:HG2   | 2:17:C:VAL:HG22 | 1        | 0.14          |
| (1,3722) | 2:1:C:MET:HG2   | 2:17:C:VAL:HG23 | 1        | 0.14          |
| (1,3722) | 2:1:C:MET:HG3   | 2:17:C:VAL:HG21 | 1        | 0.14          |
| (1,3722) | 2:1:C:MET:HG3   | 2:17:C:VAL:HG22 | 1        | 0.14          |
| (1,3722) | 2:1:C:MET:HG3   | 2:17:C:VAL:HG23 | 1        | 0.14          |
| (1,3718) | 2:1:C:MET:HE1   | 2:17:C:VAL:HG23 | 6        | 0.14          |

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| Key      | Atom-1           | Atom-2          | Model ID | Violation (Å) |
|----------|------------------|-----------------|----------|---------------|
| (1,3714) | 2:1:C:MET:HE3    | 2:17:C:VAL:HB   | 9        | 0.14          |
| (1,3703) | 2:1:C:MET:HG2    | 2:3:C:ILE:HG21  | 1        | 0.14          |
| (1,3703) | 2:1:C:MET:HG2    | 2:3:C:ILE:HG22  | 1        | 0.14          |
| (1,3703) | 2:1:C:MET:HG2    | 2:3:C:ILE:HG23  | 1        | 0.14          |
| (1,3703) | 2:1:C:MET:HG3    | 2:3:C:ILE:HG21  | 1        | 0.14          |
| (1,3703) | 2:1:C:MET:HG3    | 2:3:C:ILE:HG22  | 1        | 0.14          |
| (1,3703) | 2:1:C:MET:HG3    | 2:3:C:ILE:HG23  | 1        | 0.14          |
| (1,2844) | 2:34:B:GLU:HG3   | 2:69:B:LEU:HD21 | 3        | 0.14          |
| (1,2229) | 2:20:B:SER:HB3   | 2:21:B:ASP:H    | 9        | 0.14          |
| (1,1940) | 2:14:B:THR:HG22  | 2:14:B:THR:H    | 6        | 0.14          |
| (1,1940) | 2:14:B:THR:HG22  | 2:14:B:THR:H    | 7        | 0.14          |
| (1,1940) | 2:14:B:THR:HG23  | 2:14:B:THR:H    | 8        | 0.14          |
| (1,1940) | 2:14:B:THR:HG22  | 2:14:B:THR:H    | 9        | 0.14          |
| (1,1838) | 2:6:B:LYS:HG3    | 2:66:B:THR:HG22 | 9        | 0.14          |
| (1,1767) | 2:17:B:VAL:HG11  | 2:29:B:LYS:HG3  | 7        | 0.14          |
| (1,1748) | 2:5:B:VAL:HG22   | 2:15:B:LEU:HG   | 9        | 0.14          |
| (1,1135) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HB2 | 1        | 0.14          |
| (1,1135) | 1:556:A:ILE:HG21 | 1:557:A:GLU:HB3 | 1        | 0.14          |
| (1,1135) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HB2 | 1        | 0.14          |
| (1,1135) | 1:556:A:ILE:HG22 | 1:557:A:GLU:HB3 | 1        | 0.14          |
| (1,1135) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HB2 | 1        | 0.14          |
| (1,1135) | 1:556:A:ILE:HG23 | 1:557:A:GLU:HB3 | 1        | 0.14          |
| (1,407)  | 1:547:A:MET:HE1  | 1:547:A:MET:H   | 4        | 0.14          |
| (1,407)  | 1:547:A:MET:HE2  | 1:547:A:MET:H   | 4        | 0.14          |
| (1,407)  | 1:547:A:MET:HE3  | 1:547:A:MET:H   | 4        | 0.14          |
| (3,24)   | 2:1:B:MET:HE1    | 2:67:B:LEU:HD13 | 9        | 0.13          |
| (1,5900) | 2:70:C:VAL:HG13  | 2:68:C:HIS:HB3  | 1        | 0.13          |
| (1,4206) | 2:14:C:THR:HG21  | 2:14:C:THR:H    | 5        | 0.13          |
| (1,4206) | 2:14:C:THR:HG21  | 2:14:C:THR:H    | 7        | 0.13          |
| (1,4205) | 2:12:C:THR:HG21  | 2:13:C:ILE:H    | 7        | 0.13          |
| (1,4127) | 2:7:C:THR:HG21   | 2:11:C:LYS:HD2  | 9        | 0.13          |
| (1,4127) | 2:7:C:THR:HG21   | 2:11:C:LYS:HD3  | 9        | 0.13          |
| (1,4127) | 2:7:C:THR:HG22   | 2:11:C:LYS:HD2  | 9        | 0.13          |
| (1,4127) | 2:7:C:THR:HG22   | 2:11:C:LYS:HD3  | 9        | 0.13          |
| (1,4127) | 2:7:C:THR:HG23   | 2:11:C:LYS:HD2  | 9        | 0.13          |
| (1,4127) | 2:7:C:THR:HG23   | 2:11:C:LYS:HD3  | 9        | 0.13          |
| (1,4094) | 2:11:C:LYS:HE2   | 2:13:C:ILE:HD13 | 7        | 0.13          |
| (1,3888) | 2:29:C:LYS:HA    | 2:33:C:LYS:HE2  | 10       | 0.13          |
| (1,3036) | 2:41:B:GLN:HA    | 2:71:B:LEU:HD22 | 7        | 0.13          |
| (1,1940) | 2:14:B:THR:HG23  | 2:14:B:THR:H    | 2        | 0.13          |
| (1,1883) | 2:7:B:THR:HA     | 2:69:B:LEU:HD23 | 8        | 0.13          |
| (1,1775) | 2:5:B:VAL:HA     | 2:66:B:THR:HG22 | 9        | 0.13          |

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| Key      | Atom-1          | Atom-2          | Model ID | Violation (Å) |
|----------|-----------------|-----------------|----------|---------------|
| (1,1774) | 2:5:B:VAL:HA    | 2:66:B:THR:HG22 | 9        | 0.13          |
| (1,1766) | 2:17:B:VAL:HG12 | 2:29:B:LYS:HG3  | 1        | 0.13          |
| (1,1749) | 2:5:B:VAL:HG23  | 2:13:B:ILE:HG13 | 6        | 0.13          |
| (1,1511) | 2:1:B:MET:HG3   | 2:63:B:LYS:HA   | 5        | 0.13          |
| (1,1511) | 2:1:B:MET:HG3   | 2:63:B:LYS:HA   | 6        | 0.13          |
| (1,407)  | 1:547:A:MET:HE1 | 1:547:A:MET:H   | 2        | 0.13          |
| (1,407)  | 1:547:A:MET:HE2 | 1:547:A:MET:H   | 2        | 0.13          |
| (1,407)  | 1:547:A:MET:HE3 | 1:547:A:MET:H   | 2        | 0.13          |
| (1,407)  | 1:547:A:MET:HE1 | 1:547:A:MET:H   | 6        | 0.13          |
| (1,407)  | 1:547:A:MET:HE2 | 1:547:A:MET:H   | 6        | 0.13          |
| (1,407)  | 1:547:A:MET:HE3 | 1:547:A:MET:H   | 6        | 0.13          |
| (1,407)  | 1:547:A:MET:HE1 | 1:547:A:MET:H   | 10       | 0.13          |
| (1,407)  | 1:547:A:MET:HE2 | 1:547:A:MET:H   | 10       | 0.13          |
| (1,407)  | 1:547:A:MET:HE3 | 1:547:A:MET:H   | 10       | 0.13          |
| (3,89)   | 2:27:B:LYS:HE2  | 2:69:B:LEU:HD13 | 8        | 0.12          |
| (1,5190) | 2:36:C:ILE:HG23 | 2:71:C:LEU:HD23 | 4        | 0.12          |
| (1,5185) | 2:36:C:ILE:HG23 | 2:71:C:LEU:HD23 | 6        | 0.12          |
| (1,4206) | 2:14:C:THR:HG21 | 2:14:C:THR:H    | 6        | 0.12          |
| (1,3802) | 2:2:C:GLN:HE22  | 2:14:C:THR:HG22 | 1        | 0.12          |
| (1,3740) | 2:28:C:ALA:HB1  | 2:25:C:ASN:HA   | 10       | 0.12          |
| (1,3038) | 2:41:B:GLN:HB3  | 2:69:B:LEU:HD11 | 4        | 0.12          |
| (1,3013) | 2:40:B:GLN:HB3  | 2:71:B:LEU:HD23 | 10       | 0.12          |
| (1,2876) | 2:36:B:ILE:HG22 | 2:41:B:GLN:HB2  | 5        | 0.12          |
| (1,1838) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG21 | 10       | 0.12          |
| (1,1751) | 2:5:B:VAL:HG23  | 2:13:B:ILE:HG13 | 10       | 0.12          |
| (1,1588) | 2:29:B:LYS:HA   | 2:15:B:LEU:HD11 | 6        | 0.12          |
| (1,1474) | 2:28:B:ALA:HB2  | 2:25:B:ASN:HA   | 6        | 0.12          |
| (1,122)  | 1:503:A:ASP:H   | 1:506:A:LEU:H   | 1        | 0.12          |
| (2,3)    | 1:484:A:LYS:O   | 1:488:A:ALA:H   | 2        | 0.11          |
| (1,5900) | 2:70:C:VAL:HG11 | 2:68:C:HIS:HB3  | 7        | 0.11          |
| (1,5283) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD23 | 6        | 0.11          |
| (1,5279) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD22 | 2        | 0.11          |
| (1,4104) | 2:6:C:LYS:HG3   | 2:66:C:THR:HG21 | 3        | 0.11          |
| (1,4048) | 2:5:C:VAL:HG12  | 2:69:C:LEU:HB3  | 2        | 0.11          |
| (1,4015) | 2:5:C:VAL:HG22  | 2:13:C:ILE:HG13 | 5        | 0.11          |
| (1,3775) | 2:1:C:MET:HG2   | 2:63:C:LYS:HA   | 1        | 0.11          |
| (1,3775) | 2:1:C:MET:HG3   | 2:63:C:LYS:HA   | 1        | 0.11          |
| (1,2249) | 2:52:B:ASP:HB2  | 2:24:B:GLU:HB2  | 9        | 0.11          |
| (1,1838) | 2:6:B:LYS:HG3   | 2:66:B:THR:HG22 | 4        | 0.11          |
| (1,1783) | 2:5:B:VAL:HG11  | 2:69:B:LEU:HB3  | 10       | 0.11          |
| (1,1767) | 2:17:B:VAL:HG12 | 2:29:B:LYS:HG3  | 9        | 0.11          |
| (1,1766) | 2:17:B:VAL:HG12 | 2:29:B:LYS:HG3  | 5        | 0.11          |

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| Key      | Atom-1          | Atom-2           | Model ID | Violation (Å) |
|----------|-----------------|------------------|----------|---------------|
| (1,1588) | 2:29:B:LYS:HA   | 2:15:B:LEU:HD21  | 9        | 0.11          |
| (1,1456) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG21  | 1        | 0.11          |
| (1,1456) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG22  | 1        | 0.11          |
| (1,1456) | 2:1:B:MET:HG2   | 2:17:B:VAL:HG23  | 1        | 0.11          |
| (1,1456) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG21  | 1        | 0.11          |
| (1,1456) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG22  | 1        | 0.11          |
| (1,1456) | 2:1:B:MET:HG3   | 2:17:B:VAL:HG23  | 1        | 0.11          |
| (1,1119) | 1:554:A:THR:HB  | 1:556:A:ILE:HG21 | 10       | 0.11          |
| (1,1119) | 1:554:A:THR:HB  | 1:556:A:ILE:HG22 | 10       | 0.11          |
| (1,1119) | 1:554:A:THR:HB  | 1:556:A:ILE:HG23 | 10       | 0.11          |
| (1,407)  | 1:547:A:MET:HE1 | 1:547:A:MET:H    | 5        | 0.11          |
| (1,407)  | 1:547:A:MET:HE2 | 1:547:A:MET:H    | 5        | 0.11          |
| (1,407)  | 1:547:A:MET:HE3 | 1:547:A:MET:H    | 5        | 0.11          |
| (1,225)  | 1:512:A:ILE:H   | 1:515:A:SER:H    | 9        | 0.11          |
| (1,75)   | 1:548:A:ASP:OD1 | 2:42:B:ARG:NH2   | 4        | 0.11          |
| (1,5900) | 2:70:C:VAL:HG12 | 2:68:C:HIS:HB3   | 5        | 0.1           |
| (1,5278) | 2:40:C:GLN:HB3  | 2:71:C:LEU:HD21  | 9        | 0.1           |
| (1,4515) | 2:52:C:ASP:HB2  | 2:24:C:GLU:HB2   | 4        | 0.1           |
| (1,4515) | 2:52:C:ASP:HB2  | 2:24:C:GLU:HB2   | 7        | 0.1           |
| (1,4515) | 2:52:C:ASP:HB2  | 2:24:C:GLU:HB2   | 10       | 0.1           |
| (1,4313) | 2:15:C:LEU:HD13 | 2:26:C:VAL:HA    | 5        | 0.1           |
| (1,4032) | 2:17:C:VAL:HG13 | 2:29:C:LYS:HG3   | 3        | 0.1           |
| (1,1940) | 2:14:B:THR:HG22 | 2:14:B:THR:H     | 3        | 0.1           |
| (1,1783) | 2:5:B:VAL:HG13  | 2:69:B:LEU:HB3   | 5        | 0.1           |
| (1,1474) | 2:28:B:ALA:HB2  | 2:25:B:ASN:HA    | 4        | 0.1           |
| (1,507)  | 1:575:A:MET:HE1 | 1:575:A:MET:H    | 3        | 0.1           |
| (1,507)  | 1:575:A:MET:HE2 | 1:575:A:MET:H    | 3        | 0.1           |
| (1,507)  | 1:575:A:MET:HE3 | 1:575:A:MET:H    | 3        | 0.1           |
| (1,76)   | 1:552:A:GLU:OE2 | 2:42:B:ARG:NH1   | 5        | 0.1           |

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

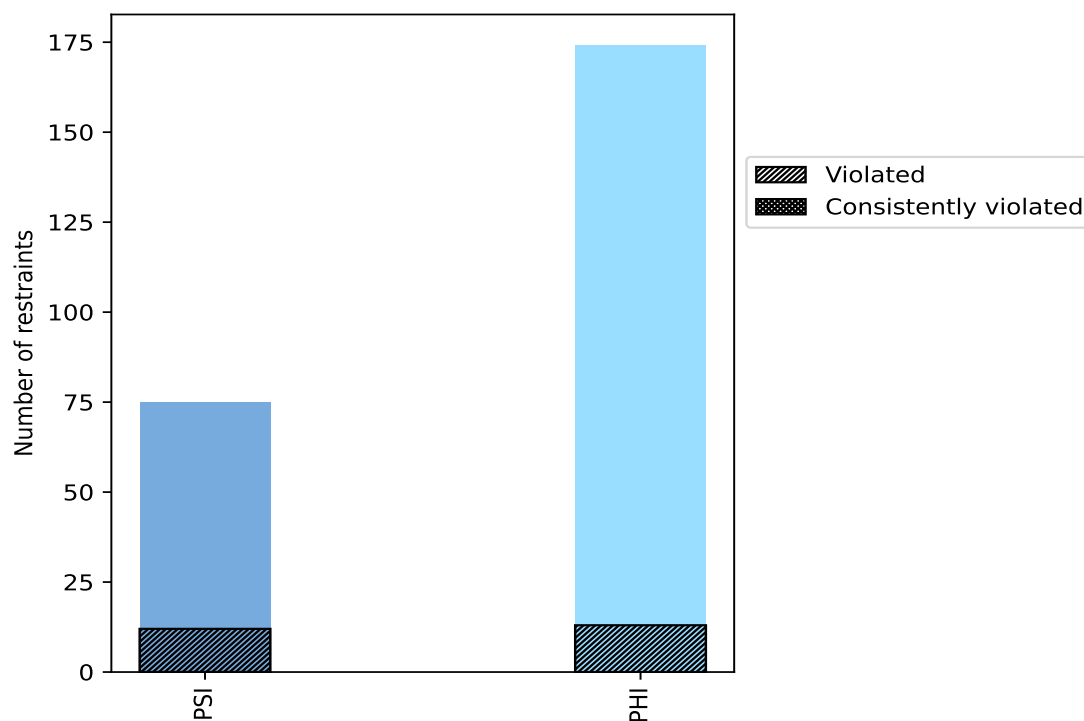
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

| Angle type | Count | % <sup>1</sup> | Violated <sup>3</sup> |                |                | Consistently Violated <sup>4</sup> |                |                |
|------------|-------|----------------|-----------------------|----------------|----------------|------------------------------------|----------------|----------------|
|            |       |                | Count                 | % <sup>2</sup> | % <sup>1</sup> | Count                              | % <sup>2</sup> | % <sup>1</sup> |
| PSI        | 75    | 30.1           | 12                    | 16.0           | 4.8            | 0                                  | 0.0            | 0.0            |
| PHI        | 174   | 69.9           | 13                    | 7.5            | 5.2            | 0                                  | 0.0            | 0.0            |
| Total      | 249   | 100.0          | 25                    | 10.0           | 10.0           | 0                                  | 0.0            | 0.0            |

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

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



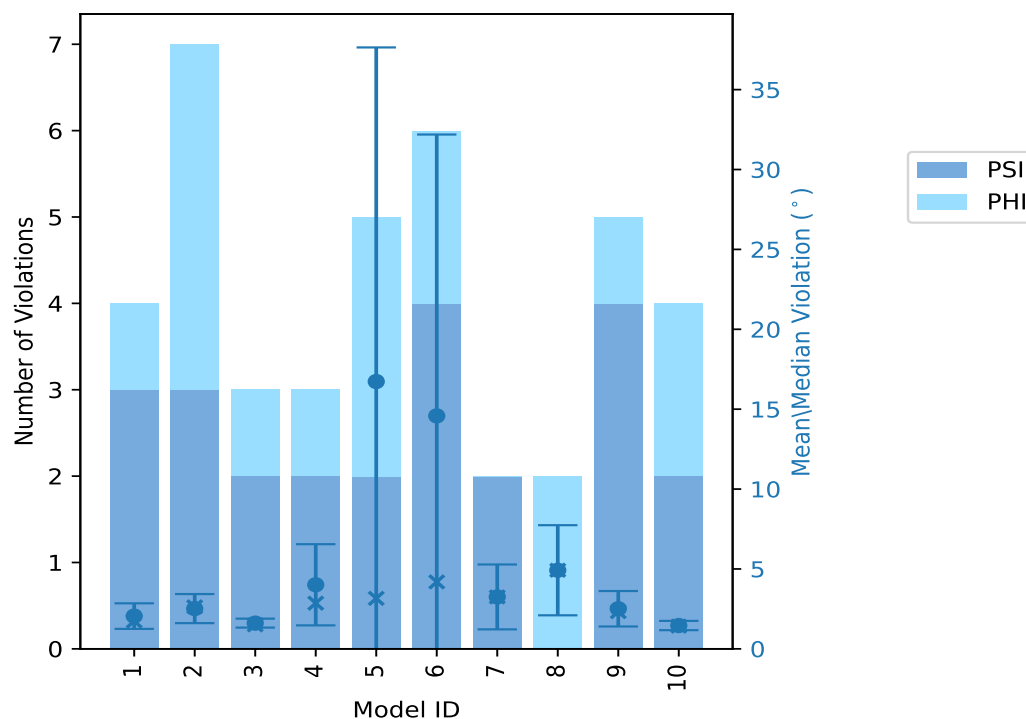
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

| Model ID | Number of violations |     |       | Mean (°) | Max (°) | SD (°) | Median (°) |
|----------|----------------------|-----|-------|----------|---------|--------|------------|
|          | PSI                  | PHI | Total |          |         |        |            |
| 1        | 3                    | 1   | 4     | 2.05     | 3.4     | 0.8    | 1.74       |
| 2        | 3                    | 4   | 7     | 2.52     | 3.7     | 0.91   | 2.63       |
| 3        | 2                    | 1   | 3     | 1.61     | 1.99    | 0.28   | 1.5        |
| 4        | 2                    | 1   | 3     | 4.01     | 7.54    | 2.54   | 2.86       |
| 5        | 2                    | 3   | 5     | 16.73    | 55.81   | 20.91  | 3.16       |
| 6        | 4                    | 2   | 6     | 14.58    | 48.49   | 17.61  | 4.19       |
| 7        | 2                    | 0   | 2     | 3.25     | 5.28    | 2.03   | 3.25       |
| 8        | 0                    | 2   | 2     | 4.92     | 7.73    | 2.82   | 4.92       |
| 9        | 4                    | 1   | 5     | 2.51     | 4.52    | 1.11   | 2.33       |
| 10       | 2                    | 2   | 4     | 1.46     | 1.9     | 0.29   | 1.42       |

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



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

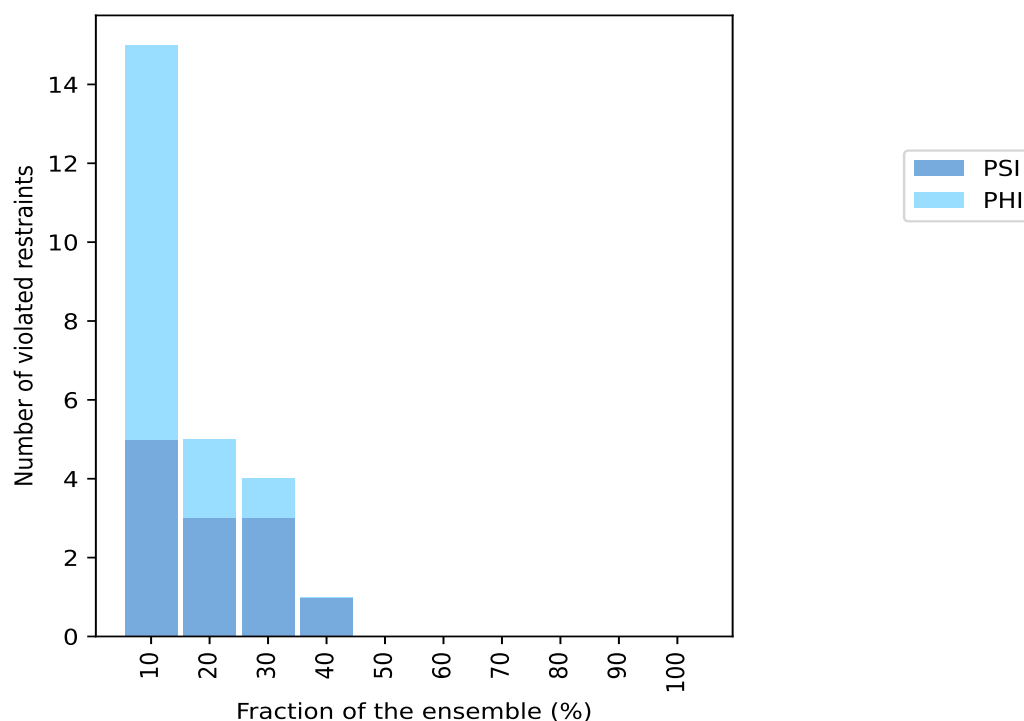
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

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

| Number of violated restraints |     |       | Fraction of the ensemble |       |
|-------------------------------|-----|-------|--------------------------|-------|
| PSI                           | PHI | Total | Count <sup>1</sup>       | %     |
| 5                             | 10  | 15    | 1                        | 10.0  |
| 3                             | 2   | 5     | 2                        | 20.0  |
| 3                             | 1   | 4     | 3                        | 30.0  |
| 1                             | 0   | 1     | 4                        | 40.0  |
| 0                             | 0   | 0     | 5                        | 50.0  |
| 0                             | 0   | 0     | 6                        | 60.0  |
| 0                             | 0   | 0     | 7                        | 70.0  |
| 0                             | 0   | 0     | 8                        | 80.0  |
| 0                             | 0   | 0     | 9                        | 90.0  |
| 0                             | 0   | 0     | 10                       | 100.0 |

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

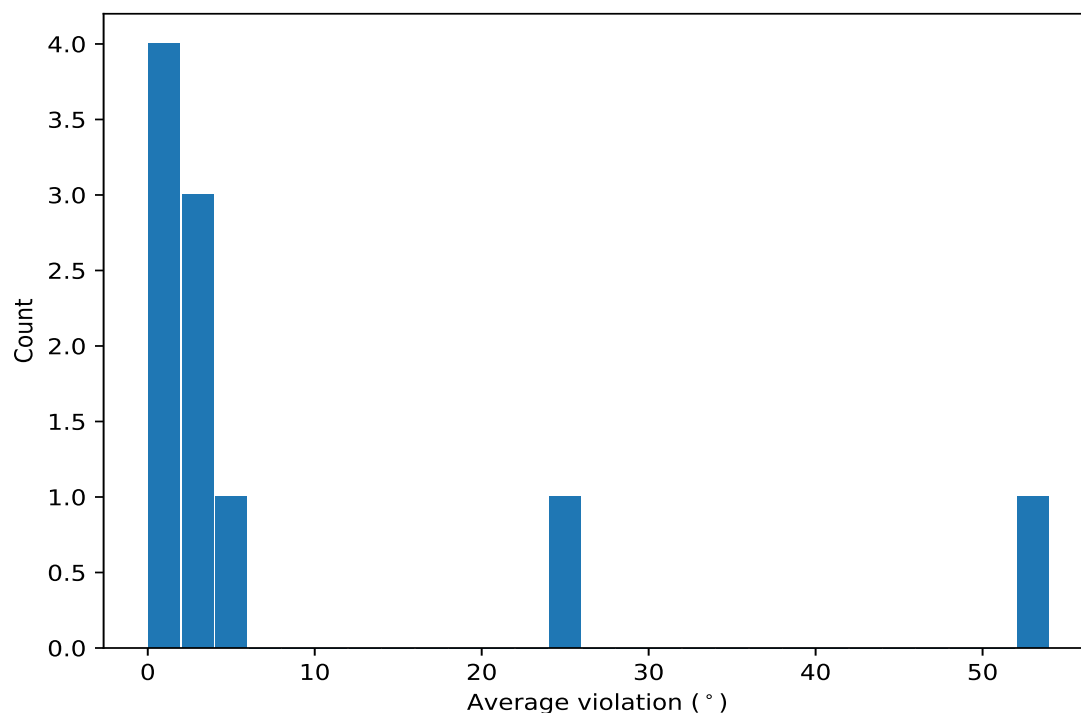
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 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.

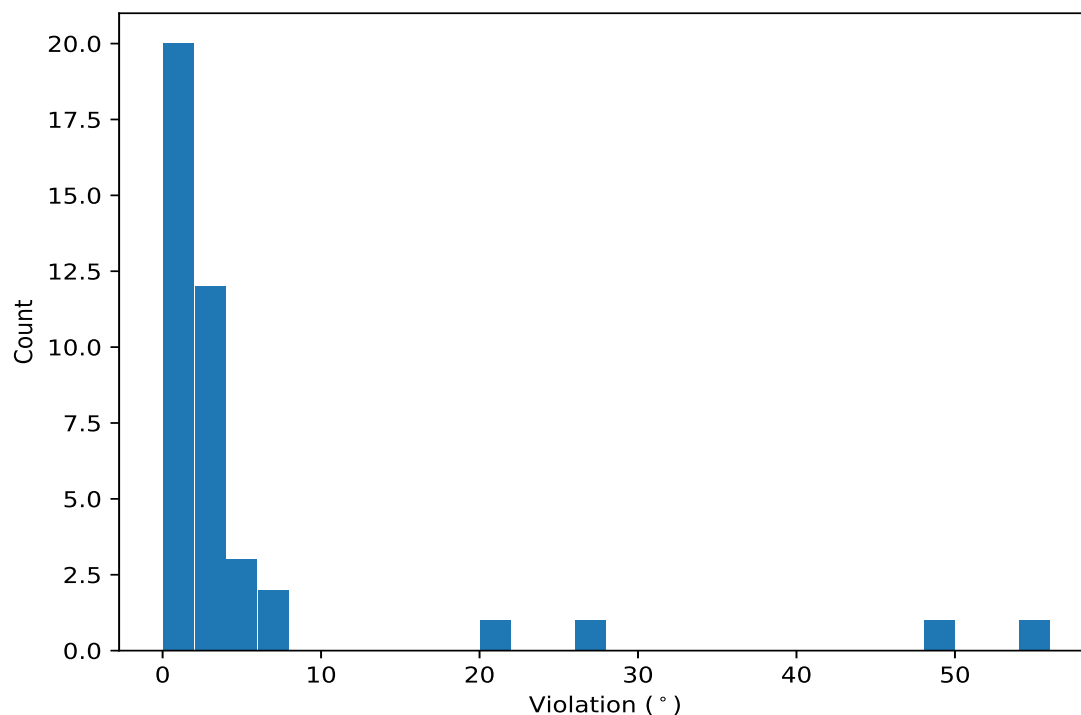
| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Models <sup>1</sup> | Mean  | SD <sup>2</sup> | Median |
|---------|---------------|----------------|----------------|---------------|---------------------|-------|-----------------|--------|
| (1,90)  | 1:551:A:LEU:N | 1:551:A:LEU:CA | 1:551:A:LEU:C  | 1:552:A:GLU:N | 4                   | 3.14  | 1.46            | 3.01   |
| (1,10)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:ALA:N | 3                   | 2.39  | 1.51            | 1.33   |
| (1,54)  | 1:528:A:LEU:C | 1:529:A:ALA:N  | 1:529:A:ALA:CA | 1:529:A:ALA:C | 3                   | 1.68  | 0.17            | 1.64   |
| (1,155) | 1:606:A:CYS:N | 1:606:A:CYS:CA | 1:606:A:CYS:C  | 1:607:A:ALA:N | 3                   | 1.67  | 0.24            | 1.61   |
| (1,111) | 1:571:A:GLY:N | 1:571:A:GLY:CA | 1:571:A:GLY:C  | 1:572:A:ILE:N | 3                   | 1.18  | 0.04            | 1.19   |
| (1,117) | 1:578:A:GLY:C | 1:579:A:GLU:N  | 1:579:A:GLU:CA | 1:579:A:GLU:C | 2                   | 52.15 | 3.66            | 52.15  |
| (1,118) | 1:579:A:GLU:N | 1:579:A:GLU:CA | 1:579:A:GLU:C  | 1:580:A:GLN:N | 2                   | 24.3  | 2.97            | 24.3   |
| (1,15)  | 1:503:A:ASP:N | 1:503:A:ASP:CA | 1:503:A:ASP:C  | 1:504:A:GLU:N | 2                   | 5.08  | 2.46            | 5.08   |
| (1,75)  | 1:543:A:THR:C | 1:544:A:THR:N  | 1:544:A:THR:CA | 1:544:A:THR:C | 2                   | 3.92  | 0.75            | 3.92   |
| (1,141) | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:SER:N | 2                   | 1.78  | 0.11            | 1.78   |

<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 (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,117) | 1:578:A:GLY:C | 1:579:A:GLU:N  | 1:579:A:GLU:CA | 1:579:A:GLU:C | 5        | 55.81         |
| (1,117) | 1:578:A:GLY:C | 1:579:A:GLU:N  | 1:579:A:GLU:CA | 1:579:A:GLU:C | 6        | 48.49         |
| (1,118) | 1:579:A:GLU:N | 1:579:A:GLU:CA | 1:579:A:GLU:C  | 1:580:A:GLN:N | 6        | 27.27         |
| (1,118) | 1:579:A:GLU:N | 1:579:A:GLU:CA | 1:579:A:GLU:C  | 1:580:A:GLN:N | 5        | 21.33         |
| (1,139) | 1:594:A:PRO:C | 1:595:A:MET:N  | 1:595:A:MET:CA | 1:595:A:MET:C | 8        | 7.73          |
| (1,15)  | 1:503:A:ASP:N | 1:503:A:ASP:CA | 1:503:A:ASP:C  | 1:504:A:GLU:N | 4        | 7.54          |
| (1,90)  | 1:551:A:LEU:N | 1:551:A:LEU:CA | 1:551:A:LEU:C  | 1:552:A:GLU:N | 7        | 5.28          |
| (1,75)  | 1:543:A:THR:C | 1:544:A:THR:N  | 1:544:A:THR:CA | 1:544:A:THR:C | 6        | 4.67          |
| (1,10)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:ALA:N | 9        | 4.52          |
| (1,160) | 2:6:B:LYS:C   | 2:7:B:THR:N    | 2:7:B:THR:CA   | 2:7:B:THR:C   | 2        | 3.7           |
| (1,38)  | 1:519:A:PRO:N | 1:519:A:PRO:CA | 1:519:A:PRO:C  | 1:520:A:ILE:N | 6        | 3.7           |
| (1,90)  | 1:551:A:LEU:N | 1:551:A:LEU:CA | 1:551:A:LEU:C  | 1:552:A:GLU:N | 1        | 3.4           |
| (1,14)  | 1:502:A:ASN:C | 1:503:A:ASP:N  | 1:503:A:ASP:CA | 1:503:A:ASP:C | 2        | 3.38          |
| (1,24)  | 1:507:A:GLY:C | 1:508:A:LEU:N  | 1:508:A:LEU:CA | 1:508:A:LEU:C | 2        | 3.33          |

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| Key     | Atom-1        | Atom-2         | Atom-3         | Atom-4        | Model ID | Violation (°) |
|---------|---------------|----------------|----------------|---------------|----------|---------------|
| (1,75)  | 1:543:A:THR:C | 1:544:A:THR:N  | 1:544:A:THR:CA | 1:544:A:THR:C | 5        | 3.16          |
| (1,4)   | 1:489:A:ALA:N | 1:489:A:ALA:CA | 1:489:A:ALA:C  | 1:490:A:ILE:N | 4        | 2.86          |
| (1,90)  | 1:551:A:LEU:N | 1:551:A:LEU:CA | 1:551:A:LEU:C  | 1:552:A:GLU:N | 9        | 2.63          |
| (1,15)  | 1:503:A:ASP:N | 1:503:A:ASP:CA | 1:503:A:ASP:C  | 1:504:A:GLU:N | 2        | 2.63          |
| (1,13)  | 1:498:A:ALA:C | 1:499:A:GLY:N  | 1:499:A:GLY:CA | 1:499:A:GLY:C | 9        | 2.33          |
| (1,55)  | 1:529:A:ALA:N | 1:529:A:ALA:CA | 1:529:A:ALA:C  | 1:530:A:LEU:N | 6        | 2.23          |
| (1,116) | 1:573:A:LEU:C | 1:574:A:TYR:N  | 1:574:A:TYR:CA | 1:574:A:TYR:C | 8        | 2.1           |
| (1,155) | 1:606:A:CYS:N | 1:606:A:CYS:CA | 1:606:A:CYS:C  | 1:607:A:ALA:N | 3        | 1.99          |
| (1,200) | 2:67:B:LEU:C  | 2:68:B:HIS:N   | 2:68:B:HIS:CA  | 2:68:B:HIS:C  | 5        | 1.94          |
| (1,54)  | 1:528:A:LEU:C | 1:529:A:ALA:N  | 1:529:A:ALA:CA | 1:529:A:ALA:C | 10       | 1.9           |
| (1,141) | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:SER:N | 9        | 1.89          |
| (1,203) | 2:2:C:GLN:C   | 2:3:C:ILE:N    | 2:3:C:ILE:CA   | 2:3:C:ILE:C   | 1        | 1.82          |
| (1,67)  | 1:539:A:ASN:C | 1:540:A:GLY:N  | 1:540:A:GLY:CA | 1:540:A:GLY:C | 2        | 1.79          |
| (1,141) | 1:596:A:THR:N | 1:596:A:THR:CA | 1:596:A:THR:C  | 1:597:A:SER:N | 1        | 1.67          |
| (1,54)  | 1:528:A:LEU:C | 1:529:A:ALA:N  | 1:529:A:ALA:CA | 1:529:A:ALA:C | 4        | 1.64          |
| (1,155) | 1:606:A:CYS:N | 1:606:A:CYS:CA | 1:606:A:CYS:C  | 1:607:A:ALA:N | 2        | 1.61          |
| (1,12)  | 1:498:A:ALA:N | 1:498:A:ALA:CA | 1:498:A:ALA:C  | 1:499:A:GLY:N | 10       | 1.55          |
| (1,54)  | 1:528:A:LEU:C | 1:529:A:ALA:N  | 1:529:A:ALA:CA | 1:529:A:ALA:C | 3        | 1.5           |
| (1,155) | 1:606:A:CYS:N | 1:606:A:CYS:CA | 1:606:A:CYS:C  | 1:607:A:ALA:N | 5        | 1.42          |
| (1,10)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:ALA:N | 3        | 1.33          |
| (1,10)  | 1:497:A:PHE:N | 1:497:A:PHE:CA | 1:497:A:PHE:C  | 1:498:A:ALA:N | 1        | 1.31          |
| (1,156) | 2:2:B:GLN:C   | 2:3:B:ILE:N    | 2:3:B:ILE:CA   | 2:3:B:ILE:C   | 10       | 1.29          |
| (1,90)  | 1:551:A:LEU:N | 1:551:A:LEU:CA | 1:551:A:LEU:C  | 1:552:A:GLU:N | 2        | 1.23          |
| (1,111) | 1:571:A:GLY:N | 1:571:A:GLY:CA | 1:571:A:GLY:C  | 1:572:A:ILE:N | 7        | 1.22          |
| (1,111) | 1:571:A:GLY:N | 1:571:A:GLY:CA | 1:571:A:GLY:C  | 1:572:A:ILE:N | 9        | 1.19          |
| (1,111) | 1:571:A:GLY:N | 1:571:A:GLY:CA | 1:571:A:GLY:C  | 1:572:A:ILE:N | 6        | 1.12          |
| (1,27)  | 1:509:A:LEU:N | 1:509:A:LEU:CA | 1:509:A:LEU:C  | 1:510:A:LEU:N | 10       | 1.12          |