



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:32 pm GMT

PDB ID : 2JXY  
Title : Solution structure of the hemopexin-like domain of MMP12  
Authors : Bertini, I.; Calderone, V.; Fragai, M.; Jaiswal, R.; Luchinat, C.; Melikian, M.  
Deposited on : 2007-12-01

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

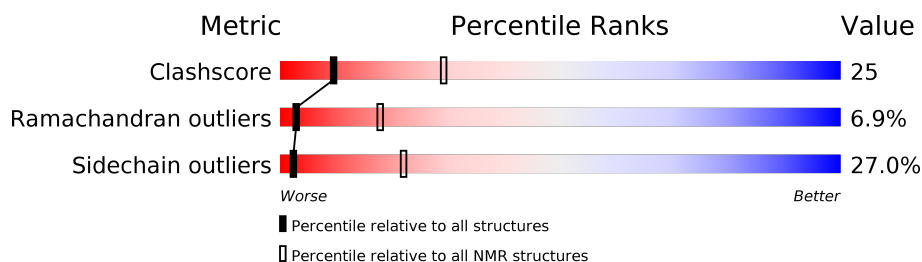
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 79%.

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            | 125131                      | 11601                     |
| Ramachandran outliers | 121729                      | 10391                     |
| Sidechain outliers    | 121581                      | 10367                     |

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     | 194    |  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:281-A:470 (190)     | 0.70              | 1            |

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

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

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

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

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

There are 2 unique types of molecules in this entry. The entry contains 3243 atoms, of which 1595 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Macrophage metalloelastase.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
| 1   | A     | 194      | Total | C    | H    | N   | O   | S | 0     |
|     |       |          | 3242  | 1089 | 1595 | 267 | 286 | 5 |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 277     | MET      | -      | EXPRESSION TAG | UNP P39900 |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

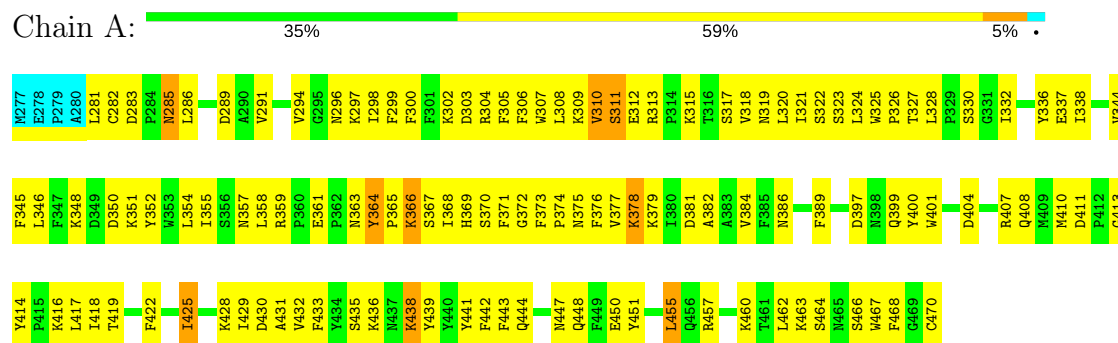
| Mol | Chain | Residues | Atoms |    |
|-----|-------|----------|-------|----|
| 2   | A     | 1        | Total | Ca |
|     |       |          | 1     | 1  |

## 4 Residue-property plots

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

These plots are provided for all protein, RNA and DNA 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: Macrophage metalloelastase

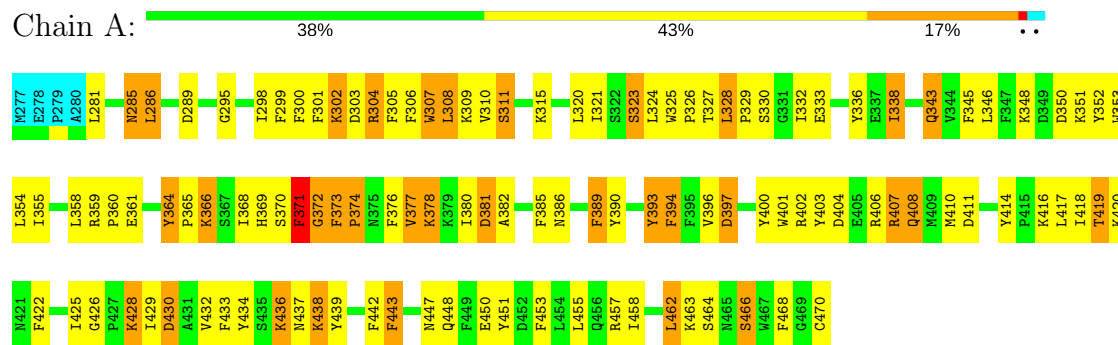


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

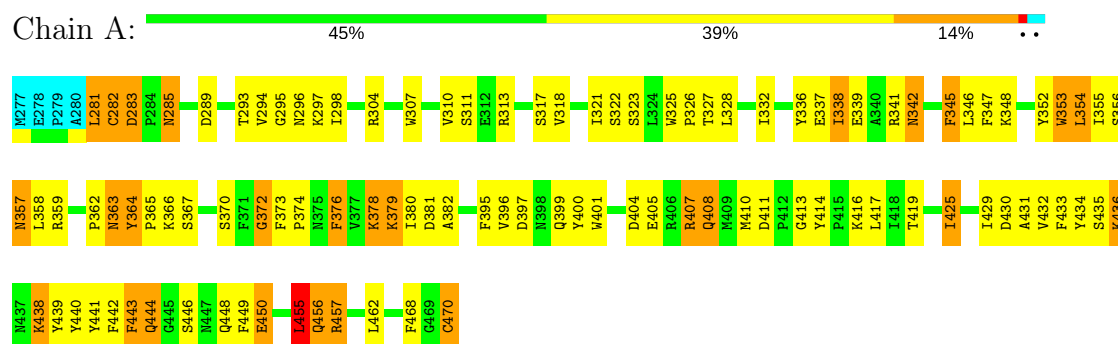
- Molecule 1: Macrophage metalloelastase





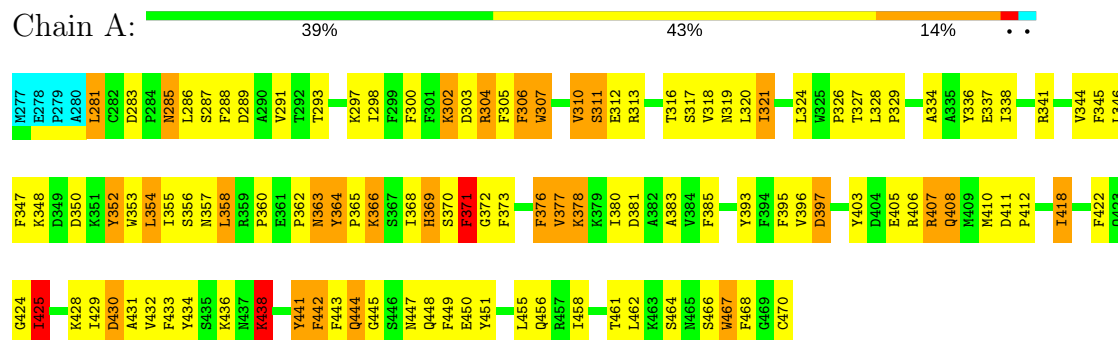
### 4.2.5 Score per residue for model 5

- Molecule 1: Macrophage metalloelastase



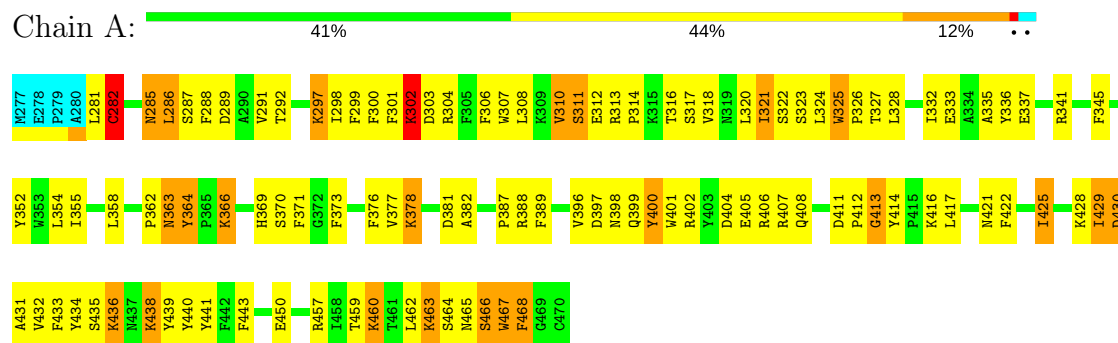
### 4.2.6 Score per residue for model 6

- Molecule 1: Macrophage metalloelastase



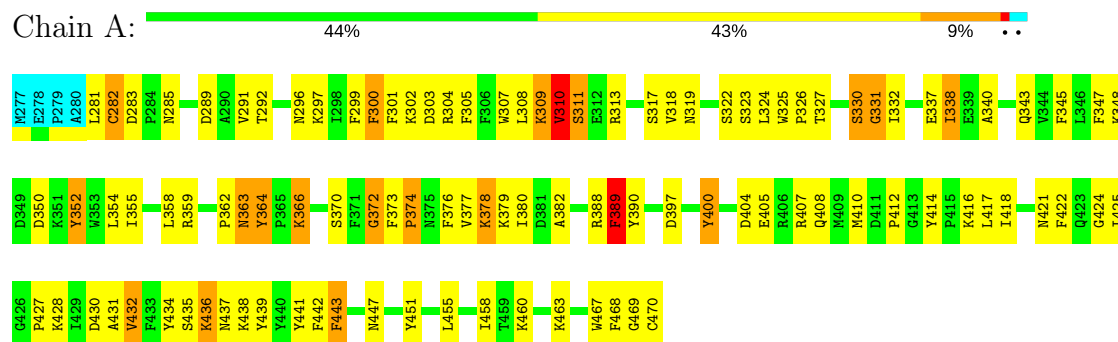
### 4.2.7 Score per residue for model 7

- Molecule 1: Macrophage metalloelastase



### 4.2.8 Score per residue for model 8

- Molecule 1: Macrophage metalloelastase





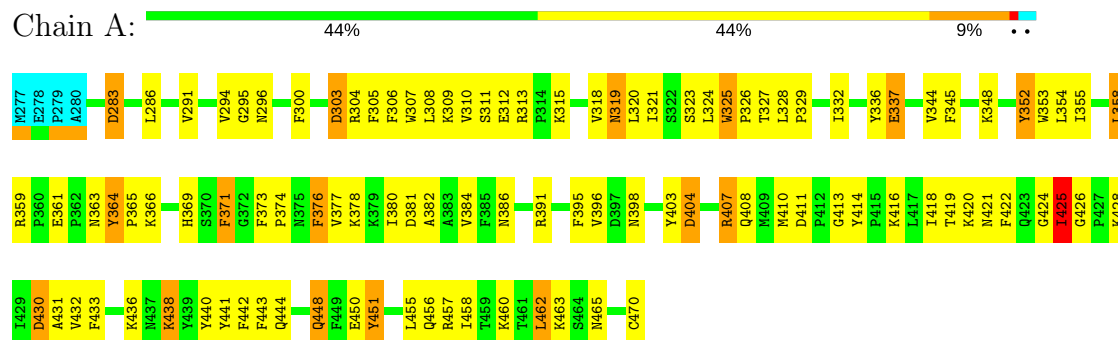
### 4.2.11 Score per residue for model 11

- Molecule 1: Macrophage metalloelastase



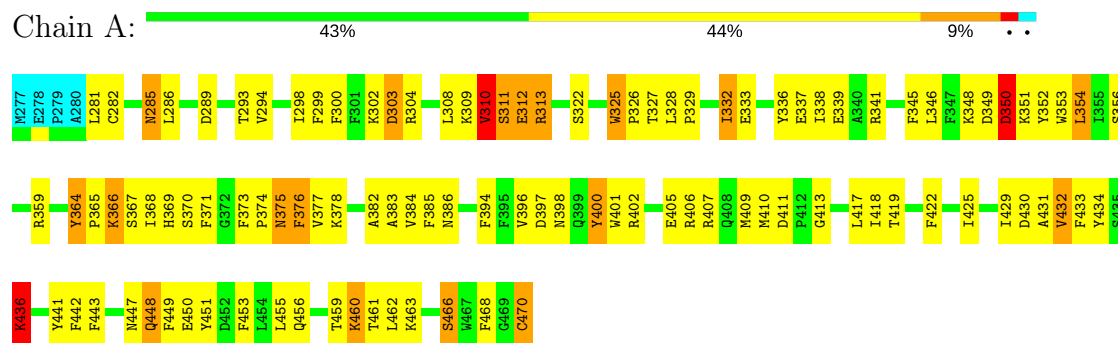
### 4.2.12 Score per residue for model 12

- Molecule 1: Macrophage metalloelastase



### 4.2.13 Score per residue for model 13

- Molecule 1: Macrophage metalloelastase



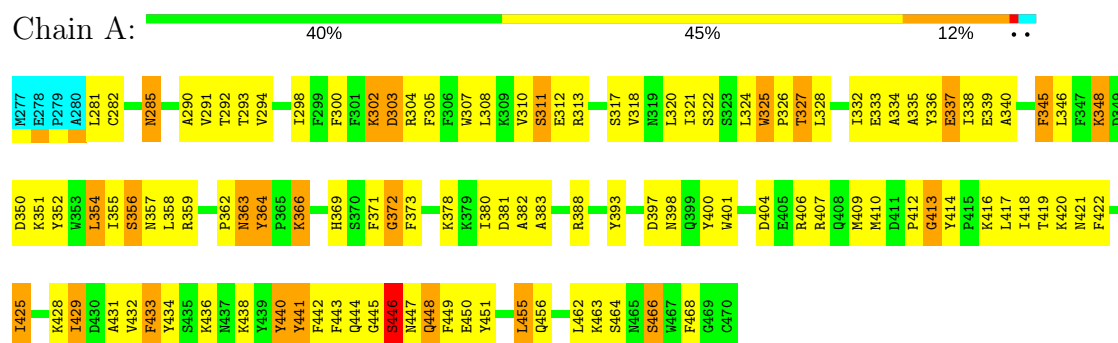
## 4.2.14 Score per residue for model 14

- Molecule 1: Macrophage metalloelastase



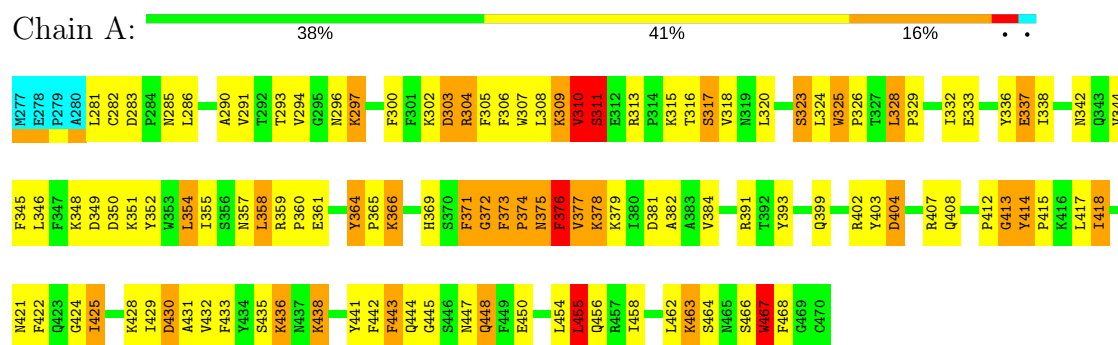
## 4.2.15 Score per residue for model 15

- Molecule 1: Macrophage metalloelastase



## 4.2.16 Score per residue for model 16

- Molecule 1: Macrophage metalloelastase



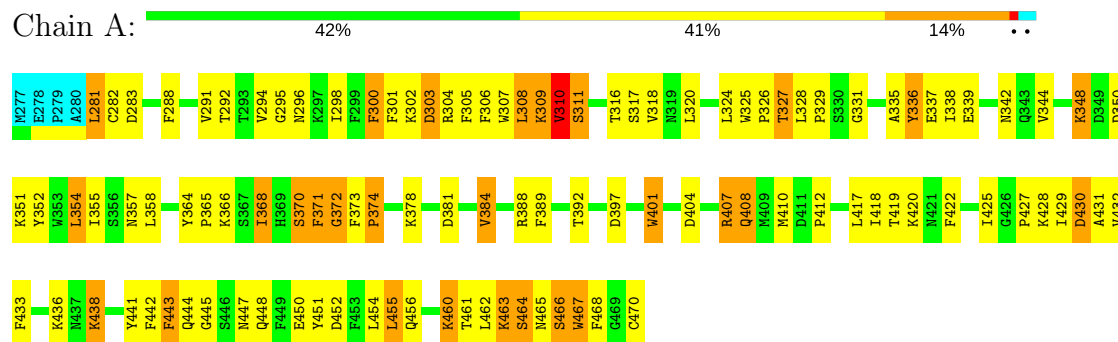
## 4.2.17 Score per residue for model 17

- Molecule 1: Macrophage metalloelastase



## 4.2.18 Score per residue for model 18

- Molecule 1: Macrophage metalloelastase



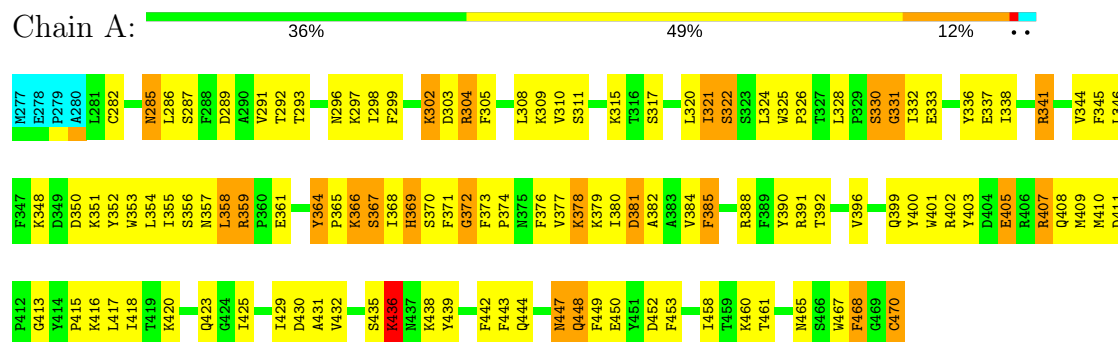
## 4.2.19 Score per residue for model 19

- Molecule 1: Macrophage metalloelastase



## 4.2.20 Score per residue for model 20

## ● Molecule 1: Macrophage metalloelastase



## 5 Refinement protocol and experimental data overview

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

Of the 1600 calculated structures, 20 were deposited, based on the following criterion: *lowest target function*.

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

| Software name | Classification | Version |
|---------------|----------------|---------|
| DYANA         | refinement     |         |

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

|  |                                   |
|--|-----------------------------------|
| Chemical shift file(s)                       | BMRB entry 7414, BMRB entry 15578 |
| Number of chemical shift lists               | 2                                 |
| Total number of shifts                       | 5866                              |
| Number of shifts mapped to atoms             | 4253                              |
| Number of unparsed shifts                    | 0                                 |
| Number of shifts with mapping errors         | 1613                              |
| Number of shifts with mapping warnings       | 0                                 |
| Assignment completeness (well-defined parts) | 79%                               |

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 1618  | 1568     | 1565     | 80±15   |
| All | All   | 32380 | 31360    | 31324    | 1602    |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:CZ3  | 1.00     | 1.91        | 17     | 1     |
| 1:A:328:LEU:HD21 | 1:A:355:ILE:HD11 | 0.94     | 1.40        | 10     | 3     |
| 1:A:346:LEU:HD23 | 1:A:355:ILE:HD13 | 0.92     | 1.37        | 2      | 2     |
| 1:A:291:VAL:HG21 | 1:A:442:PHE:CZ   | 0.91     | 2.01        | 15     | 1     |
| 1:A:298:ILE:HD13 | 1:A:300:PHE:CZ   | 0.90     | 2.01        | 13     | 1     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CE1  | 0.88     | 2.02        | 8      | 3     |
| 1:A:368:ILE:HD12 | 1:A:377:VAL:HG13 | 0.88     | 1.45        | 2      | 1     |
| 1:A:286:LEU:HD11 | 1:A:307:TRP:CZ2  | 0.88     | 2.04        | 16     | 2     |
| 1:A:336:TYR:OH   | 1:A:338:ILE:HD11 | 0.87     | 1.69        | 10     | 1     |
| 1:A:327:THR:O    | 1:A:328:LEU:HD22 | 0.87     | 1.70        | 6      | 13    |
| 1:A:334:ALA:HB1  | 1:A:383:ALA:HB2  | 0.86     | 1.46        | 15     | 1     |
| 1:A:281:LEU:HD11 | 1:A:316:THR:OG1  | 0.85     | 1.71        | 18     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:450:GLU:O    | 1:A:458:ILE:HG23 | 0.84     | 1.72        | 1      | 3     |
| 1:A:382:ALA:HB1  | 1:A:432:VAL:HG12 | 0.84     | 1.50        | 1      | 5     |
| 1:A:354:LEU:HD23 | 1:A:364:TYR:CE2  | 0.83     | 2.08        | 18     | 3     |
| 1:A:350:ASP:O    | 1:A:368:ILE:HG23 | 0.82     | 1.74        | 13     | 1     |
| 1:A:338:ILE:HD12 | 1:A:345:PHE:CE1  | 0.82     | 2.10        | 10     | 2     |
| 1:A:291:VAL:HG22 | 1:A:431:ALA:HB1  | 0.81     | 1.50        | 4      | 5     |
| 1:A:291:VAL:HG21 | 1:A:442:PHE:CE1  | 0.81     | 2.11        | 15     | 1     |
| 1:A:291:VAL:HG21 | 1:A:300:PHE:CE2  | 0.80     | 2.11        | 16     | 1     |
| 1:A:424:GLY:CA   | 1:A:458:ILE:HD11 | 0.80     | 2.06        | 12     | 2     |
| 1:A:337:GLU:OE1  | 1:A:344:VAL:HG22 | 0.80     | 1.75        | 19     | 1     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:CB   | 0.79     | 2.07        | 15     | 3     |
| 1:A:364:TYR:N    | 1:A:365:PRO:CD   | 0.79     | 2.46        | 12     | 3     |
| 1:A:328:LEU:HD13 | 1:A:329:PRO:HD2  | 0.79     | 1.54        | 10     | 6     |
| 1:A:290:ALA:HB2  | 1:A:333:GLU:O    | 0.78     | 1.77        | 15     | 2     |
| 1:A:429:ILE:HD11 | 1:A:440:TYR:OH   | 0.78     | 1.77        | 15     | 1     |
| 1:A:336:TYR:CZ   | 1:A:338:ILE:HD11 | 0.77     | 2.14        | 10     | 1     |
| 1:A:347:PHE:CZ   | 1:A:380:ILE:HD12 | 0.77     | 2.15        | 5      | 1     |
| 1:A:288:PHE:CE2  | 1:A:300:PHE:CD1  | 0.77     | 2.72        | 4      | 2     |
| 1:A:281:LEU:HD13 | 1:A:316:THR:OG1  | 0.77     | 1.80        | 17     | 1     |
| 1:A:396:VAL:HG22 | 1:A:397:ASP:OD1  | 0.76     | 1.79        | 19     | 1     |
| 1:A:298:ILE:HD12 | 1:A:310:VAL:HG23 | 0.76     | 1.58        | 20     | 1     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:CB   | 0.74     | 2.10        | 13     | 7     |
| 1:A:449:PHE:CE1  | 1:A:461:THR:HG22 | 0.74     | 2.16        | 14     | 1     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:HB3  | 0.74     | 1.57        | 1      | 7     |
| 1:A:347:PHE:CE1  | 1:A:380:ILE:HD12 | 0.74     | 2.18        | 5      | 1     |
| 1:A:432:VAL:HG23 | 1:A:441:TYR:O    | 0.73     | 1.82        | 16     | 2     |
| 1:A:299:PHE:CD1  | 1:A:308:LEU:HD23 | 0.73     | 2.18        | 9      | 1     |
| 1:A:425:ILE:HD13 | 1:A:425:ILE:N    | 0.72     | 2.00        | 10     | 3     |
| 1:A:425:ILE:N    | 1:A:425:ILE:HD13 | 0.72     | 1.99        | 6      | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CD2  | 0.72     | 2.20        | 16     | 2     |
| 1:A:281:LEU:HD21 | 1:A:307:TRP:CD1  | 0.72     | 2.20        | 5      | 1     |
| 1:A:354:LEU:HD12 | 1:A:355:ILE:N    | 0.72     | 1.98        | 8      | 5     |
| 1:A:346:LEU:HD23 | 1:A:355:ILE:CD1  | 0.71     | 2.16        | 2      | 1     |
| 1:A:334:ALA:HB1  | 1:A:383:ALA:CB   | 0.71     | 2.15        | 15     | 2     |
| 1:A:297:LYS:HA   | 1:A:310:VAL:HG11 | 0.71     | 1.62        | 5      | 3     |
| 1:A:354:LEU:C    | 1:A:354:LEU:HD12 | 0.71     | 2.05        | 18     | 2     |
| 1:A:345:PHE:C    | 1:A:346:LEU:HD23 | 0.71     | 2.05        | 10     | 1     |
| 1:A:345:PHE:C    | 1:A:346:LEU:HD22 | 0.70     | 2.06        | 2      | 8     |
| 1:A:384:VAL:HG11 | 1:A:432:VAL:HG12 | 0.70     | 1.62        | 18     | 1     |
| 1:A:425:ILE:CG2  | 1:A:429:ILE:HD13 | 0.70     | 2.17        | 5      | 1     |
| 1:A:428:LYS:C    | 1:A:429:ILE:HD12 | 0.70     | 2.07        | 1      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:298:ILE:O    | 1:A:298:ILE:HD12 | 0.69     | 1.86        | 13     | 1     |
| 1:A:353:TRP:NE1  | 1:A:364:TYR:CE1  | 0.69     | 2.60        | 12     | 1     |
| 1:A:396:VAL:HG12 | 1:A:397:ASP:OD2  | 0.69     | 1.88        | 6      | 1     |
| 1:A:281:LEU:HD13 | 1:A:468:PHE:CE2  | 0.69     | 2.23        | 1      | 1     |
| 1:A:418:ILE:HG22 | 1:A:425:ILE:HD11 | 0.69     | 1.63        | 14     | 2     |
| 1:A:346:LEU:N    | 1:A:346:LEU:HD23 | 0.69     | 2.03        | 10     | 1     |
| 1:A:354:LEU:HD12 | 1:A:354:LEU:C    | 0.68     | 2.08        | 19     | 1     |
| 1:A:297:LYS:HA   | 1:A:310:VAL:HG21 | 0.68     | 1.65        | 20     | 4     |
| 1:A:382:ALA:HB1  | 1:A:432:VAL:HG22 | 0.68     | 1.64        | 14     | 3     |
| 1:A:304:ARG:O    | 1:A:320:LEU:HD12 | 0.68     | 1.89        | 20     | 1     |
| 1:A:424:GLY:HA3  | 1:A:458:ILE:HD11 | 0.68     | 1.64        | 12     | 3     |
| 1:A:429:ILE:HD11 | 1:A:442:PHE:HB3  | 0.68     | 1.66        | 3      | 3     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:HB3  | 0.67     | 1.65        | 15     | 1     |
| 1:A:432:VAL:CG2  | 1:A:442:PHE:CE1  | 0.67     | 2.77        | 1      | 2     |
| 1:A:461:THR:O    | 1:A:461:THR:HG22 | 0.67     | 1.89        | 6      | 2     |
| 1:A:364:TYR:C    | 1:A:364:TYR:CD1  | 0.67     | 2.67        | 12     | 1     |
| 1:A:354:LEU:HD13 | 1:A:354:LEU:C    | 0.67     | 2.09        | 17     | 1     |
| 1:A:346:LEU:CD2  | 1:A:355:ILE:HD13 | 0.67     | 2.18        | 2      | 1     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CZ   | 0.67     | 2.24        | 8      | 2     |
| 1:A:357:ASN:O    | 1:A:358:LEU:HD23 | 0.67     | 1.88        | 4      | 5     |
| 1:A:418:ILE:HD13 | 1:A:427:PRO:O    | 0.67     | 1.90        | 18     | 2     |
| 1:A:281:LEU:HD23 | 1:A:307:TRP:CH2  | 0.66     | 2.25        | 19     | 2     |
| 1:A:327:THR:C    | 1:A:328:LEU:HD22 | 0.66     | 2.09        | 9      | 6     |
| 1:A:354:LEU:HD23 | 1:A:354:LEU:O    | 0.66     | 1.90        | 13     | 2     |
| 1:A:328:LEU:HD11 | 1:A:346:LEU:HD11 | 0.66     | 1.66        | 10     | 1     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:HB3  | 0.66     | 1.67        | 15     | 1     |
| 1:A:399:GLN:O    | 1:A:418:ILE:HD11 | 0.65     | 1.91        | 20     | 5     |
| 1:A:338:ILE:HD11 | 1:A:385:PHE:HB3  | 0.65     | 1.66        | 20     | 1     |
| 1:A:281:LEU:HD13 | 1:A:468:PHE:CD2  | 0.65     | 2.26        | 1      | 1     |
| 1:A:421:ASN:ND2  | 1:A:422:PHE:CZ   | 0.65     | 2.65        | 15     | 1     |
| 1:A:281:LEU:CD2  | 1:A:468:PHE:CD1  | 0.65     | 2.79        | 11     | 1     |
| 1:A:299:PHE:CE2  | 1:A:308:LEU:HD23 | 0.65     | 2.26        | 8      | 2     |
| 1:A:433:PHE:CE1  | 1:A:443:PHE:CZ   | 0.65     | 2.85        | 7      | 1     |
| 1:A:443:PHE:CE2  | 1:A:448:GLN:NE2  | 0.64     | 2.65        | 2      | 3     |
| 1:A:373:PHE:O    | 1:A:373:PHE:CD2  | 0.64     | 2.50        | 20     | 2     |
| 1:A:328:LEU:HD11 | 1:A:355:ILE:HD11 | 0.64     | 1.66        | 14     | 2     |
| 1:A:299:PHE:CD2  | 1:A:308:LEU:HD21 | 0.64     | 2.27        | 3      | 1     |
| 1:A:291:VAL:HG23 | 1:A:299:PHE:O    | 0.64     | 1.93        | 7      | 1     |
| 1:A:382:ALA:HB2  | 1:A:431:ALA:HA   | 0.64     | 1.69        | 16     | 5     |
| 1:A:432:VAL:HG13 | 1:A:441:TYR:O    | 0.64     | 1.93        | 12     | 1     |
| 1:A:310:VAL:HG13 | 1:A:311:SER:N    | 0.64     | 2.08        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:327:THR:HG23 | 1:A:327:THR:O    | 0.64     | 1.93        | 2      | 4     |
| 1:A:384:VAL:CG2  | 1:A:432:VAL:HG13 | 0.63     | 2.23        | 10     | 2     |
| 1:A:449:PHE:CE2  | 1:A:461:THR:CG2  | 0.63     | 2.81        | 20     | 1     |
| 1:A:336:TYR:CE2  | 1:A:338:ILE:HD11 | 0.63     | 2.28        | 2      | 1     |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:CG   | 0.63     | 2.81        | 15     | 2     |
| 1:A:355:ILE:N    | 1:A:355:ILE:HD12 | 0.63     | 2.09        | 11     | 4     |
| 1:A:281:LEU:CD2  | 1:A:468:PHE:CE1  | 0.63     | 2.82        | 11     | 1     |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:CB   | 0.63     | 2.81        | 9      | 2     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CD2  | 0.63     | 2.87        | 16     | 1     |
| 1:A:369:HIS:NE2  | 1:A:373:PHE:CD1  | 0.63     | 2.66        | 16     | 1     |
| 1:A:336:TYR:CE1  | 1:A:345:PHE:CB   | 0.63     | 2.81        | 2      | 3     |
| 1:A:384:VAL:O    | 1:A:392:THR:HG23 | 0.63     | 1.93        | 20     | 6     |
| 1:A:338:ILE:HD12 | 1:A:345:PHE:CD1  | 0.63     | 2.28        | 10     | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CG   | 0.62     | 2.87        | 16     | 1     |
| 1:A:443:PHE:CD2  | 1:A:448:GLN:NE2  | 0.62     | 2.67        | 2      | 1     |
| 1:A:307:TRP:CD1  | 1:A:317:SER:O    | 0.62     | 2.52        | 18     | 1     |
| 1:A:291:VAL:HG22 | 1:A:431:ALA:CB   | 0.62     | 2.23        | 20     | 1     |
| 1:A:328:LEU:HD21 | 1:A:360:PRO:HG3  | 0.62     | 1.71        | 9      | 1     |
| 1:A:298:ILE:H    | 1:A:310:VAL:HG11 | 0.62     | 1.55        | 15     | 4     |
| 1:A:364:TYR:N    | 1:A:365:PRO:HD2  | 0.62     | 2.10        | 12     | 1     |
| 1:A:332:ILE:HG23 | 1:A:347:PHE:O    | 0.62     | 1.94        | 5      | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CG   | 0.62     | 2.30        | 17     | 1     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:CD1  | 0.62     | 2.29        | 11     | 1     |
| 1:A:316:THR:CG2  | 1:A:468:PHE:CD1  | 0.62     | 2.82        | 6      | 1     |
| 1:A:400:TYR:O    | 1:A:400:TYR:CD1  | 0.61     | 2.53        | 20     | 1     |
| 1:A:425:ILE:HG22 | 1:A:429:ILE:HD13 | 0.61     | 1.71        | 5      | 1     |
| 1:A:338:ILE:O    | 1:A:338:ILE:HG23 | 0.61     | 1.95        | 4      | 5     |
| 1:A:448:GLN:NE2  | 1:A:462:LEU:HD21 | 0.61     | 2.09        | 13     | 1     |
| 1:A:422:PHE:O    | 1:A:425:ILE:HD11 | 0.61     | 1.95        | 6      | 2     |
| 1:A:338:ILE:HG23 | 1:A:338:ILE:O    | 0.61     | 1.95        | 13     | 3     |
| 1:A:434:TYR:CD2  | 1:A:434:TYR:O    | 0.61     | 2.53        | 6      | 2     |
| 1:A:298:ILE:HD13 | 1:A:300:PHE:CE2  | 0.61     | 2.31        | 13     | 1     |
| 1:A:325:TRP:HB3  | 1:A:328:LEU:HD23 | 0.61     | 1.72        | 9      | 8     |
| 1:A:329:PRO:O    | 1:A:332:ILE:HD11 | 0.61     | 1.94        | 12     | 1     |
| 1:A:282:CYS:SG   | 1:A:470:CYS:CB   | 0.61     | 2.89        | 5      | 1     |
| 1:A:467:TRP:O    | 1:A:468:PHE:CD1  | 0.61     | 2.54        | 18     | 1     |
| 1:A:395:PHE:CE2  | 1:A:432:VAL:HG21 | 0.61     | 2.30        | 14     | 1     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:OG   | 0.61     | 1.95        | 2      | 2     |
| 1:A:294:VAL:HG23 | 1:A:297:LYS:HB2  | 0.61     | 1.72        | 14     | 1     |
| 1:A:291:VAL:HG11 | 1:A:443:PHE:CE1  | 0.61     | 2.31        | 6      | 1     |
| 1:A:316:THR:HG22 | 1:A:468:PHE:CD1  | 0.61     | 2.31        | 6      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:308:LEU:HD23 | 1:A:309:LYS:N    | 0.61     | 2.10        | 20     | 1     |
| 1:A:299:PHE:CE1  | 1:A:308:LEU:HD23 | 0.61     | 2.30        | 9      | 1     |
| 1:A:429:ILE:HD11 | 1:A:442:PHE:CD1  | 0.60     | 2.31        | 16     | 2     |
| 1:A:327:THR:O    | 1:A:327:THR:HG23 | 0.60     | 1.96        | 12     | 4     |
| 1:A:361:GLU:OE2  | 1:A:364:TYR:CE1  | 0.60     | 2.54        | 3      | 1     |
| 1:A:332:ILE:HG13 | 1:A:346:LEU:HD12 | 0.60     | 1.74        | 14     | 1     |
| 1:A:368:ILE:HD12 | 1:A:377:VAL:CG1  | 0.60     | 2.25        | 2      | 1     |
| 1:A:337:GLU:HG2  | 1:A:344:VAL:HG22 | 0.60     | 1.74        | 6      | 1     |
| 1:A:297:LYS:HA   | 1:A:310:VAL:HG23 | 0.60     | 1.73        | 19     | 3     |
| 1:A:294:VAL:HG22 | 1:A:337:GLU:CD   | 0.60     | 2.16        | 17     | 1     |
| 1:A:361:GLU:OE1  | 1:A:364:TYR:CE1  | 0.60     | 2.54        | 10     | 1     |
| 1:A:332:ILE:HD13 | 1:A:346:LEU:HD12 | 0.60     | 1.72        | 5      | 2     |
| 1:A:286:LEU:CD1  | 1:A:307:TRP:CZ2  | 0.60     | 2.83        | 16     | 1     |
| 1:A:403:TYR:CE1  | 1:A:404:ASP:O    | 0.60     | 2.55        | 12     | 3     |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:CG   | 0.60     | 2.90        | 2      | 1     |
| 1:A:298:ILE:CD1  | 1:A:310:VAL:HG23 | 0.60     | 2.27        | 20     | 1     |
| 1:A:336:TYR:CD1  | 1:A:336:TYR:C    | 0.59     | 2.75        | 18     | 2     |
| 1:A:305:PHE:CE1  | 1:A:320:LEU:HD12 | 0.59     | 2.31        | 4      | 3     |
| 1:A:347:PHE:CD1  | 1:A:347:PHE:N    | 0.59     | 2.70        | 10     | 1     |
| 1:A:466:SER:O    | 1:A:467:TRP:CD1  | 0.59     | 2.55        | 19     | 2     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:OE1  | 0.59     | 2.55        | 6      | 2     |
| 1:A:400:TYR:CE1  | 1:A:401:TRP:O    | 0.59     | 2.55        | 5      | 2     |
| 1:A:372:GLY:O    | 1:A:373:PHE:C    | 0.59     | 2.40        | 11     | 10    |
| 1:A:389:PHE:C    | 1:A:390:TYR:CG   | 0.59     | 2.75        | 14     | 4     |
| 1:A:336:TYR:C    | 1:A:336:TYR:CD1  | 0.59     | 2.75        | 3      | 1     |
| 1:A:293:THR:HG21 | 1:A:434:TYR:O    | 0.59     | 1.97        | 5      | 1     |
| 1:A:358:LEU:HD23 | 1:A:359:ARG:HG2  | 0.59     | 1.73        | 17     | 1     |
| 1:A:441:TYR:N    | 1:A:441:TYR:CD1  | 0.59     | 2.68        | 15     | 1     |
| 1:A:361:GLU:OE1  | 1:A:364:TYR:CD1  | 0.59     | 2.55        | 10     | 1     |
| 1:A:281:LEU:O    | 1:A:468:PHE:CZ   | 0.59     | 2.55        | 5      | 1     |
| 1:A:354:LEU:C    | 1:A:355:ILE:HD12 | 0.59     | 2.18        | 15     | 3     |
| 1:A:438:LYS:O    | 1:A:439:TYR:CD1  | 0.59     | 2.55        | 14     | 3     |
| 1:A:296:ASN:O    | 1:A:310:VAL:HG21 | 0.59     | 1.98        | 8      | 2     |
| 1:A:421:ASN:O    | 1:A:422:PHE:CD1  | 0.59     | 2.56        | 2      | 2     |
| 1:A:306:PHE:CD1  | 1:A:306:PHE:O    | 0.59     | 2.56        | 7      | 1     |
| 1:A:432:VAL:HG22 | 1:A:442:PHE:HB3  | 0.59     | 1.75        | 6      | 1     |
| 1:A:395:PHE:CD2  | 1:A:429:ILE:HG21 | 0.59     | 2.33        | 2      | 3     |
| 1:A:368:ILE:CD1  | 1:A:377:VAL:HG21 | 0.59     | 2.28        | 9      | 1     |
| 1:A:462:LEU:HD22 | 1:A:466:SER:HB2  | 0.58     | 1.73        | 10     | 1     |
| 1:A:336:TYR:CG   | 1:A:336:TYR:O    | 0.58     | 2.56        | 18     | 7     |
| 1:A:443:PHE:CD1  | 1:A:443:PHE:C    | 0.58     | 2.75        | 1      | 4     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:281:LEU:HD21 | 1:A:468:PHE:CE1  | 0.58     | 2.33        | 11     | 1     |
| 1:A:346:LEU:HD22 | 1:A:346:LEU:N    | 0.58     | 2.13        | 2      | 2     |
| 1:A:299:PHE:CZ   | 1:A:308:LEU:HD23 | 0.58     | 2.34        | 13     | 1     |
| 1:A:377:VAL:HG22 | 1:A:396:VAL:HG11 | 0.58     | 1.76        | 13     | 1     |
| 1:A:425:ILE:HG22 | 1:A:442:PHE:CZ   | 0.58     | 2.33        | 20     | 1     |
| 1:A:382:ALA:HB3  | 1:A:432:VAL:HG12 | 0.58     | 1.75        | 4      | 1     |
| 1:A:290:ALA:HB2  | 1:A:333:GLU:C    | 0.58     | 2.19        | 15     | 1     |
| 1:A:290:ALA:HB2  | 1:A:332:ILE:O    | 0.58     | 1.97        | 10     | 1     |
| 1:A:286:LEU:CD2  | 1:A:288:PHE:CZ   | 0.58     | 2.86        | 10     | 1     |
| 1:A:298:ILE:HD11 | 1:A:309:LYS:O    | 0.58     | 1.98        | 13     | 1     |
| 1:A:396:VAL:HG21 | 1:A:401:TRP:CZ3  | 0.58     | 2.33        | 20     | 1     |
| 1:A:421:ASN:OD1  | 1:A:422:PHE:CE2  | 0.58     | 2.57        | 7      | 4     |
| 1:A:372:GLY:O    | 1:A:373:PHE:CD2  | 0.58     | 2.57        | 6      | 1     |
| 1:A:294:VAL:O    | 1:A:294:VAL:HG23 | 0.58     | 1.98        | 18     | 2     |
| 1:A:352:TYR:CD1  | 1:A:352:TYR:C    | 0.58     | 2.77        | 12     | 1     |
| 1:A:454:LEU:HD23 | 1:A:455:LEU:CD2  | 0.58     | 2.29        | 16     | 1     |
| 1:A:357:ASN:C    | 1:A:358:LEU:HD23 | 0.57     | 2.19        | 2      | 2     |
| 1:A:288:PHE:CD2  | 1:A:300:PHE:CE1  | 0.57     | 2.92        | 18     | 1     |
| 1:A:352:TYR:C    | 1:A:352:TYR:CD1  | 0.57     | 2.76        | 8      | 3     |
| 1:A:364:TYR:CD2  | 1:A:365:PRO:HD3  | 0.57     | 2.34        | 12     | 1     |
| 1:A:334:ALA:HB1  | 1:A:383:ALA:HB3  | 0.57     | 1.74        | 10     | 2     |
| 1:A:434:TYR:CG   | 1:A:434:TYR:O    | 0.57     | 2.57        | 6      | 2     |
| 1:A:373:PHE:CZ   | 1:A:375:ASN:O    | 0.57     | 2.57        | 17     | 1     |
| 1:A:352:TYR:CD1  | 1:A:368:ILE:HG23 | 0.57     | 2.34        | 19     | 2     |
| 1:A:380:ILE:HG23 | 1:A:395:PHE:O    | 0.57     | 1.98        | 5      | 1     |
| 1:A:425:ILE:HD13 | 1:A:425:ILE:H    | 0.57     | 1.58        | 19     | 4     |
| 1:A:307:TRP:CZ3  | 1:A:468:PHE:CE1  | 0.57     | 2.92        | 7      | 1     |
| 1:A:300:PHE:N    | 1:A:300:PHE:CD1  | 0.57     | 2.73        | 8      | 2     |
| 1:A:401:TRP:CH2  | 1:A:411:ASP:O    | 0.57     | 2.57        | 9      | 1     |
| 1:A:281:LEU:O    | 1:A:468:PHE:CE1  | 0.57     | 2.57        | 5      | 1     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CE2  | 0.57     | 2.35        | 5      | 2     |
| 1:A:328:LEU:HD12 | 1:A:346:LEU:HD12 | 0.57     | 1.76        | 4      | 1     |
| 1:A:343:GLN:NE2  | 1:A:354:LEU:HD21 | 0.57     | 2.15        | 3      | 2     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CZ   | 0.57     | 2.87        | 6      | 1     |
| 1:A:309:LYS:HB2  | 1:A:316:THR:HG22 | 0.57     | 1.76        | 16     | 1     |
| 1:A:362:PRO:O    | 1:A:363:ASN:CB   | 0.57     | 2.53        | 6      | 9     |
| 1:A:292:THR:HG21 | 1:A:337:GLU:CD   | 0.57     | 2.20        | 3      | 1     |
| 1:A:332:ILE:HD12 | 1:A:346:LEU:HB3  | 0.57     | 1.75        | 16     | 1     |
| 1:A:316:THR:HG21 | 1:A:468:PHE:CE2  | 0.57     | 2.35        | 18     | 1     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:CB   | 0.57     | 2.30        | 15     | 1     |
| 1:A:400:TYR:C    | 1:A:400:TYR:CD1  | 0.57     | 2.78        | 10     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:468:PHE:CD1  | 1:A:468:PHE:C    | 0.57     | 2.79        | 3      | 2     |
| 1:A:337:GLU:CB   | 1:A:344:VAL:HA   | 0.57     | 2.29        | 18     | 1     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:CB   | 0.57     | 2.88        | 9      | 3     |
| 1:A:332:ILE:CG2  | 1:A:335:ALA:HB2  | 0.56     | 2.30        | 2      | 1     |
| 1:A:309:LYS:HG2  | 1:A:316:THR:HG22 | 0.56     | 1.77        | 18     | 1     |
| 1:A:281:LEU:HD22 | 1:A:468:PHE:CE2  | 0.56     | 2.34        | 14     | 1     |
| 1:A:330:SER:O    | 1:A:331:GLY:C    | 0.56     | 2.42        | 8      | 2     |
| 1:A:373:PHE:CD2  | 1:A:373:PHE:O    | 0.56     | 2.58        | 19     | 1     |
| 1:A:306:PHE:CD2  | 1:A:319:ASN:O    | 0.56     | 2.58        | 12     | 2     |
| 1:A:467:TRP:O    | 1:A:468:PHE:CG   | 0.56     | 2.58        | 7      | 2     |
| 1:A:384:VAL:HB   | 1:A:432:VAL:HG23 | 0.56     | 1.76        | 19     | 2     |
| 1:A:327:THR:HG22 | 1:A:327:THR:O    | 0.56     | 2.00        | 1      | 1     |
| 1:A:301:PHE:CD1  | 1:A:332:ILE:HD13 | 0.56     | 2.35        | 11     | 2     |
| 1:A:298:ILE:HG21 | 1:A:300:PHE:CZ   | 0.56     | 2.35        | 9      | 1     |
| 1:A:441:TYR:CE1  | 1:A:450:GLU:CG   | 0.56     | 2.88        | 10     | 2     |
| 1:A:373:PHE:O    | 1:A:373:PHE:CG   | 0.56     | 2.56        | 20     | 1     |
| 1:A:292:THR:HG21 | 1:A:337:GLU:OE1  | 0.56     | 2.00        | 3      | 1     |
| 1:A:281:LEU:CD2  | 1:A:307:TRP:CH2  | 0.56     | 2.88        | 19     | 1     |
| 1:A:328:LEU:HD13 | 1:A:329:PRO:CD   | 0.56     | 2.29        | 16     | 3     |
| 1:A:370:SER:O    | 1:A:371:PHE:CG   | 0.56     | 2.59        | 1      | 3     |
| 1:A:382:ALA:CB   | 1:A:432:VAL:HG12 | 0.56     | 2.31        | 20     | 7     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:CD   | 0.56     | 2.78        | 10     | 2     |
| 1:A:434:TYR:O    | 1:A:434:TYR:CG   | 0.56     | 2.58        | 15     | 2     |
| 1:A:425:ILE:CD1  | 1:A:425:ILE:N    | 0.56     | 2.68        | 10     | 3     |
| 1:A:353:TRP:CH2  | 1:A:365:PRO:HA   | 0.56     | 2.35        | 5      | 1     |
| 1:A:433:PHE:O    | 1:A:433:PHE:CD1  | 0.56     | 2.59        | 15     | 2     |
| 1:A:371:PHE:CG   | 1:A:371:PHE:O    | 0.56     | 2.58        | 15     | 2     |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:CE3  | 0.56     | 2.33        | 17     | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CD1  | 0.56     | 2.94        | 16     | 1     |
| 1:A:294:VAL:HG22 | 1:A:337:GLU:OE1  | 0.56     | 2.00        | 15     | 1     |
| 1:A:332:ILE:HG21 | 1:A:346:LEU:HD12 | 0.56     | 1.78        | 11     | 3     |
| 1:A:364:TYR:CD1  | 1:A:366:LYS:CE   | 0.56     | 2.88        | 4      | 3     |
| 1:A:336:TYR:OH   | 1:A:345:PHE:CD2  | 0.56     | 2.59        | 9      | 1     |
| 1:A:288:PHE:CE1  | 1:A:443:PHE:CZ   | 0.55     | 2.93        | 18     | 1     |
| 1:A:453:PHE:CD1  | 1:A:453:PHE:O    | 0.55     | 2.60        | 4      | 2     |
| 1:A:369:HIS:C    | 1:A:369:HIS:CD2  | 0.55     | 2.79        | 20     | 4     |
| 1:A:443:PHE:CE2  | 1:A:448:GLN:CG   | 0.55     | 2.89        | 20     | 1     |
| 1:A:299:PHE:CE2  | 1:A:308:LEU:HD21 | 0.55     | 2.36        | 11     | 2     |
| 1:A:325:TRP:CH2  | 1:A:346:LEU:HD21 | 0.55     | 2.36        | 19     | 1     |
| 1:A:336:TYR:O    | 1:A:336:TYR:CG   | 0.55     | 2.60        | 16     | 5     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CE2  | 0.55     | 2.94        | 16     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:307:TRP:CZ3  | 1:A:468:PHE:CE2  | 0.55     | 2.95        | 6      | 1     |
| 1:A:293:THR:HG22 | 1:A:298:ILE:HG22 | 0.55     | 1.78        | 5      | 1     |
| 1:A:443:PHE:C    | 1:A:443:PHE:CD1  | 0.55     | 2.79        | 19     | 1     |
| 1:A:432:VAL:CG2  | 1:A:442:PHE:CZ   | 0.55     | 2.90        | 1      | 1     |
| 1:A:299:PHE:CE2  | 1:A:308:LEU:CD2  | 0.55     | 2.90        | 11     | 2     |
| 1:A:462:LEU:HD21 | 1:A:466:SER:OG   | 0.55     | 2.00        | 2      | 1     |
| 1:A:347:PHE:CD2  | 1:A:352:TYR:CB   | 0.55     | 2.90        | 10     | 1     |
| 1:A:372:GLY:O    | 1:A:373:PHE:CG   | 0.55     | 2.59        | 6      | 1     |
| 1:A:288:PHE:CD2  | 1:A:300:PHE:CD1  | 0.55     | 2.95        | 18     | 2     |
| 1:A:301:PHE:CD2  | 1:A:332:ILE:CG1  | 0.55     | 2.90        | 7      | 1     |
| 1:A:364:TYR:CG   | 1:A:365:PRO:HD3  | 0.55     | 2.37        | 12     | 1     |
| 1:A:354:LEU:C    | 1:A:354:LEU:HD13 | 0.55     | 2.22        | 3      | 2     |
| 1:A:286:LEU:HD22 | 1:A:307:TRP:CZ2  | 0.55     | 2.37        | 2      | 1     |
| 1:A:306:PHE:CD1  | 1:A:306:PHE:C    | 0.55     | 2.79        | 18     | 4     |
| 1:A:344:VAL:CG1  | 1:A:346:LEU:CD2  | 0.55     | 2.85        | 14     | 1     |
| 1:A:384:VAL:HG13 | 1:A:432:VAL:HG13 | 0.54     | 1.78        | 16     | 2     |
| 1:A:286:LEU:HD11 | 1:A:307:TRP:CH2  | 0.54     | 2.37        | 7      | 1     |
| 1:A:369:HIS:O    | 1:A:369:HIS:CD2  | 0.54     | 2.60        | 20     | 1     |
| 1:A:288:PHE:CE2  | 1:A:443:PHE:CE2  | 0.54     | 2.95        | 9      | 2     |
| 1:A:344:VAL:HG12 | 1:A:346:LEU:CD2  | 0.54     | 2.32        | 14     | 3     |
| 1:A:395:PHE:CD1  | 1:A:418:ILE:HG23 | 0.54     | 2.37        | 6      | 1     |
| 1:A:389:PHE:O    | 1:A:390:TYR:CD2  | 0.54     | 2.60        | 1      | 4     |
| 1:A:466:SER:O    | 1:A:467:TRP:CG   | 0.54     | 2.61        | 6      | 1     |
| 1:A:371:PHE:CD1  | 1:A:371:PHE:C    | 0.54     | 2.81        | 12     | 1     |
| 1:A:292:THR:HB   | 1:A:335:ALA:HB3  | 0.54     | 1.78        | 18     | 1     |
| 1:A:368:ILE:N    | 1:A:368:ILE:HD13 | 0.54     | 2.18        | 18     | 1     |
| 1:A:354:LEU:HD12 | 1:A:355:ILE:H    | 0.54     | 1.60        | 7      | 2     |
| 1:A:293:THR:HG21 | 1:A:435:SER:CB   | 0.54     | 2.32        | 9      | 3     |
| 1:A:439:TYR:CD1  | 1:A:450:GLU:OE2  | 0.54     | 2.60        | 2      | 3     |
| 1:A:301:PHE:CE2  | 1:A:332:ILE:HD13 | 0.54     | 2.38        | 1      | 1     |
| 1:A:355:ILE:CD1  | 1:A:355:ILE:N    | 0.54     | 2.70        | 1      | 2     |
| 1:A:281:LEU:CD2  | 1:A:307:TRP:CZ2  | 0.54     | 2.91        | 6      | 1     |
| 1:A:289:ASP:O    | 1:A:431:ALA:HB2  | 0.54     | 2.02        | 6      | 1     |
| 1:A:441:TYR:CE1  | 1:A:450:GLU:OE1  | 0.54     | 2.61        | 3      | 1     |
| 1:A:312:GLU:O    | 1:A:313:ARG:C    | 0.54     | 2.46        | 9      | 2     |
| 1:A:301:PHE:CE1  | 1:A:332:ILE:HD13 | 0.54     | 2.38        | 8      | 1     |
| 1:A:291:VAL:CG2  | 1:A:431:ALA:HB1  | 0.54     | 2.32        | 8      | 1     |
| 1:A:306:PHE:CD2  | 1:A:319:ASN:ND2  | 0.54     | 2.76        | 9      | 1     |
| 1:A:414:TYR:N    | 1:A:415:PRO:HD3  | 0.54     | 2.18        | 19     | 3     |
| 1:A:288:PHE:CE2  | 1:A:300:PHE:CG   | 0.54     | 2.96        | 18     | 1     |
| 1:A:444:GLN:CG   | 1:A:444:GLN:O    | 0.54     | 2.56        | 4      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:CD2  | 0.54     | 2.96        | 2      | 1     |
| 1:A:370:SER:O    | 1:A:371:PHE:CD2  | 0.53     | 2.61        | 6      | 2     |
| 1:A:352:TYR:CD1  | 1:A:352:TYR:N    | 0.53     | 2.76        | 13     | 1     |
| 1:A:412:PRO:O    | 1:A:413:GLY:C    | 0.53     | 2.46        | 16     | 1     |
| 1:A:374:PRO:O    | 1:A:375:ASN:CB   | 0.53     | 2.57        | 10     | 2     |
| 1:A:288:PHE:CG   | 1:A:443:PHE:CD2  | 0.53     | 2.96        | 18     | 1     |
| 1:A:429:ILE:CD1  | 1:A:442:PHE:CD1  | 0.53     | 2.91        | 16     | 1     |
| 1:A:455:LEU:HD23 | 1:A:455:LEU:N    | 0.53     | 2.18        | 14     | 1     |
| 1:A:336:TYR:CE1  | 1:A:345:PHE:HB3  | 0.53     | 2.39        | 9      | 1     |
| 1:A:433:PHE:C    | 1:A:433:PHE:CD1  | 0.53     | 2.81        | 17     | 1     |
| 1:A:306:PHE:C    | 1:A:307:TRP:CE3  | 0.53     | 2.82        | 18     | 1     |
| 1:A:306:PHE:C    | 1:A:306:PHE:CD1  | 0.53     | 2.82        | 1      | 2     |
| 1:A:337:GLU:HG3  | 1:A:344:VAL:HG22 | 0.53     | 1.80        | 12     | 1     |
| 1:A:463:LYS:CD   | 1:A:463:LYS:N    | 0.53     | 2.72        | 18     | 1     |
| 1:A:443:PHE:CD1  | 1:A:448:GLN:HG2  | 0.53     | 2.38        | 15     | 1     |
| 1:A:298:ILE:HD12 | 1:A:298:ILE:C    | 0.53     | 2.23        | 13     | 1     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HD2  | 0.53     | 2.38        | 17     | 6     |
| 1:A:425:ILE:H    | 1:A:425:ILE:HD13 | 0.53     | 1.61        | 10     | 1     |
| 1:A:400:TYR:CE2  | 1:A:416:LYS:HB2  | 0.53     | 2.39        | 20     | 1     |
| 1:A:323:SER:HB3  | 1:A:324:LEU:HD12 | 0.53     | 1.80        | 16     | 1     |
| 1:A:371:PHE:O    | 1:A:371:PHE:CD2  | 0.53     | 2.62        | 20     | 2     |
| 1:A:308:LEU:C    | 1:A:308:LEU:HD23 | 0.53     | 2.24        | 20     | 1     |
| 1:A:308:LEU:C    | 1:A:308:LEU:HD13 | 0.52     | 2.25        | 9      | 1     |
| 1:A:286:LEU:CD2  | 1:A:307:TRP:CZ2  | 0.52     | 2.92        | 2      | 1     |
| 1:A:336:TYR:CD2  | 1:A:338:ILE:HD11 | 0.52     | 2.39        | 2      | 1     |
| 1:A:310:VAL:HG13 | 1:A:311:SER:H    | 0.52     | 1.62        | 18     | 2     |
| 1:A:439:TYR:CG   | 1:A:450:GLU:OE2  | 0.52     | 2.63        | 2      | 1     |
| 1:A:298:ILE:HD12 | 1:A:300:PHE:CZ   | 0.52     | 2.39        | 6      | 3     |
| 1:A:431:ALA:HB3  | 1:A:442:PHE:CE2  | 0.52     | 2.40        | 15     | 1     |
| 1:A:433:PHE:CE2  | 1:A:441:TYR:HB2  | 0.52     | 2.40        | 17     | 1     |
| 1:A:364:TYR:CE2  | 1:A:366:LYS:HD3  | 0.52     | 2.40        | 17     | 5     |
| 1:A:447:ASN:OD1  | 1:A:449:PHE:CD2  | 0.52     | 2.63        | 2      | 1     |
| 1:A:299:PHE:CZ   | 1:A:308:LEU:CD2  | 0.52     | 2.92        | 13     | 1     |
| 1:A:288:PHE:CD1  | 1:A:443:PHE:CD2  | 0.52     | 2.98        | 6      | 1     |
| 1:A:310:VAL:O    | 1:A:311:SER:C    | 0.52     | 2.47        | 18     | 5     |
| 1:A:332:ILE:HD12 | 1:A:332:ILE:N    | 0.52     | 2.19        | 2      | 1     |
| 1:A:305:PHE:CD2  | 1:A:319:ASN:O    | 0.52     | 2.62        | 8      | 1     |
| 1:A:418:ILE:HD12 | 1:A:427:PRO:O    | 0.52     | 2.05        | 17     | 1     |
| 1:A:390:TYR:O    | 1:A:405:GLU:CB   | 0.52     | 2.58        | 20     | 1     |
| 1:A:328:LEU:CD1  | 1:A:346:LEU:HD11 | 0.52     | 2.33        | 10     | 1     |
| 1:A:393:TYR:CD1  | 1:A:393:TYR:N    | 0.52     | 2.76        | 6      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:336:TYR:HB2  | 1:A:383:ALA:HB3  | 0.52     | 1.82        | 4      | 1     |
| 1:A:310:VAL:HG22 | 1:A:311:SER:H    | 0.52     | 1.65        | 17     | 5     |
| 1:A:318:VAL:O    | 1:A:318:VAL:HG12 | 0.52     | 2.03        | 10     | 2     |
| 1:A:449:PHE:CE2  | 1:A:461:THR:HG23 | 0.52     | 2.40        | 20     | 1     |
| 1:A:462:LEU:CD2  | 1:A:467:TRP:CZ2  | 0.52     | 2.92        | 2      | 1     |
| 1:A:353:TRP:CZ3  | 1:A:361:GLU:O    | 0.52     | 2.63        | 20     | 2     |
| 1:A:338:ILE:HD12 | 1:A:340:ALA:HB3  | 0.52     | 1.82        | 3      | 1     |
| 1:A:433:PHE:CE2  | 1:A:441:TYR:HB3  | 0.52     | 2.40        | 3      | 1     |
| 1:A:291:VAL:CG2  | 1:A:300:PHE:CD2  | 0.52     | 2.94        | 16     | 1     |
| 1:A:400:TYR:CD1  | 1:A:400:TYR:C    | 0.52     | 2.82        | 11     | 5     |
| 1:A:449:PHE:CD1  | 1:A:449:PHE:N    | 0.52     | 2.78        | 15     | 1     |
| 1:A:336:TYR:CE1  | 1:A:347:PHE:CE2  | 0.52     | 2.98        | 9      | 1     |
| 1:A:421:ASN:ND2  | 1:A:422:PHE:CE2  | 0.52     | 2.78        | 17     | 1     |
| 1:A:462:LEU:CD1  | 1:A:466:SER:CB   | 0.51     | 2.88        | 2      | 1     |
| 1:A:400:TYR:O    | 1:A:400:TYR:CG   | 0.51     | 2.63        | 10     | 2     |
| 1:A:325:TRP:CE3  | 1:A:328:LEU:HD12 | 0.51     | 2.41        | 10     | 1     |
| 1:A:364:TYR:CD1  | 1:A:366:LYS:HE3  | 0.51     | 2.40        | 3      | 10    |
| 1:A:309:LYS:C    | 1:A:310:VAL:HG12 | 0.51     | 2.24        | 8      | 1     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:HB2  | 0.51     | 2.39        | 9      | 1     |
| 1:A:281:LEU:HD23 | 1:A:307:TRP:CZ2  | 0.51     | 2.40        | 6      | 1     |
| 1:A:337:GLU:CG   | 1:A:344:VAL:HG22 | 0.51     | 2.36        | 12     | 2     |
| 1:A:384:VAL:HG11 | 1:A:432:VAL:CG1  | 0.51     | 2.35        | 12     | 1     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:CG   | 0.51     | 2.98        | 3      | 1     |
| 1:A:281:LEU:HD23 | 1:A:307:TRP:CZ3  | 0.51     | 2.40        | 19     | 1     |
| 1:A:328:LEU:HD11 | 1:A:346:LEU:CD1  | 0.51     | 2.36        | 16     | 1     |
| 1:A:310:VAL:HG13 | 1:A:312:GLU:H    | 0.51     | 1.66        | 11     | 1     |
| 1:A:364:TYR:CD1  | 1:A:366:LYS:HE2  | 0.51     | 2.40        | 4      | 3     |
| 1:A:307:TRP:CZ3  | 1:A:318:VAL:N    | 0.51     | 2.78        | 15     | 1     |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:HG3  | 0.51     | 2.40        | 15     | 1     |
| 1:A:281:LEU:O    | 1:A:282:CYS:CB   | 0.51     | 2.59        | 14     | 2     |
| 1:A:364:TYR:CG   | 1:A:366:LYS:CE   | 0.51     | 2.94        | 1      | 1     |
| 1:A:395:PHE:CE1  | 1:A:418:ILE:HG23 | 0.51     | 2.41        | 6      | 1     |
| 1:A:462:LEU:CG   | 1:A:466:SER:OG   | 0.51     | 2.59        | 2      | 1     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:HG3  | 0.51     | 2.40        | 16     | 2     |
| 1:A:310:VAL:O    | 1:A:313:ARG:CD   | 0.51     | 2.59        | 13     | 1     |
| 1:A:348:LYS:O    | 1:A:349:ASP:C    | 0.51     | 2.49        | 13     | 1     |
| 1:A:468:PHE:CD1  | 1:A:468:PHE:N    | 0.51     | 2.74        | 17     | 1     |
| 1:A:400:TYR:CE2  | 1:A:416:LYS:CB   | 0.51     | 2.94        | 20     | 1     |
| 1:A:422:PHE:O    | 1:A:425:ILE:CD1  | 0.51     | 2.59        | 2      | 6     |
| 1:A:364:TYR:CE2  | 1:A:366:LYS:HG3  | 0.51     | 2.41        | 18     | 1     |
| 1:A:286:LEU:CD1  | 1:A:307:TRP:CH2  | 0.51     | 2.93        | 7      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:301:PHE:CE2  | 1:A:332:ILE:HG13 | 0.51     | 2.41        | 7      | 1     |
| 1:A:374:PRO:HG2  | 1:A:377:VAL:HG13 | 0.51     | 1.82        | 8      | 1     |
| 1:A:354:LEU:HD11 | 1:A:356:SER:OG   | 0.51     | 2.06        | 10     | 1     |
| 1:A:357:ASN:O    | 1:A:358:LEU:CD2  | 0.51     | 2.59        | 16     | 5     |
| 1:A:364:TYR:N    | 1:A:365:PRO:HD3  | 0.51     | 2.21        | 20     | 12    |
| 1:A:347:PHE:CG   | 1:A:380:ILE:HD12 | 0.51     | 2.41        | 8      | 1     |
| 1:A:364:TYR:CE1  | 1:A:366:LYS:HE3  | 0.51     | 2.41        | 3      | 1     |
| 1:A:338:ILE:O    | 1:A:338:ILE:CG2  | 0.51     | 2.59        | 5      | 3     |
| 1:A:347:PHE:CZ   | 1:A:380:ILE:CD1  | 0.50     | 2.94        | 5      | 1     |
| 1:A:461:THR:C    | 1:A:462:LEU:HD13 | 0.50     | 2.27        | 19     | 1     |
| 1:A:355:ILE:HD12 | 1:A:355:ILE:N    | 0.50     | 2.20        | 10     | 2     |
| 1:A:449:PHE:CZ   | 1:A:461:THR:HG23 | 0.50     | 2.41        | 20     | 1     |
| 1:A:337:GLU:CD   | 1:A:344:VAL:HG22 | 0.50     | 2.26        | 19     | 1     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:CD   | 0.50     | 2.94        | 9      | 4     |
| 1:A:389:PHE:O    | 1:A:390:TYR:CB   | 0.50     | 2.59        | 14     | 4     |
| 1:A:367:SER:O    | 1:A:370:SER:CB   | 0.50     | 2.59        | 20     | 1     |
| 1:A:391:ARG:CG   | 1:A:392:THR:N    | 0.50     | 2.74        | 20     | 1     |
| 1:A:442:PHE:CZ   | 1:A:449:PHE:CB   | 0.50     | 2.94        | 20     | 1     |
| 1:A:394:PHE:CD1  | 1:A:403:TYR:CD1  | 0.50     | 2.99        | 4      | 1     |
| 1:A:387:PRO:HG3  | 1:A:434:TYR:CE2  | 0.50     | 2.41        | 7      | 1     |
| 1:A:399:GLN:OE1  | 1:A:415:PRO:CB   | 0.50     | 2.60        | 20     | 1     |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:HG2  | 0.50     | 2.41        | 2      | 2     |
| 1:A:291:VAL:HG12 | 1:A:300:PHE:HA   | 0.50     | 1.82        | 15     | 2     |
| 1:A:453:PHE:CD1  | 1:A:453:PHE:C    | 0.50     | 2.84        | 13     | 1     |
| 1:A:328:LEU:HD11 | 1:A:355:ILE:HG12 | 0.50     | 1.83        | 12     | 1     |
| 1:A:350:ASP:O    | 1:A:351:LYS:CG   | 0.50     | 2.60        | 15     | 10    |
| 1:A:422:PHE:HB2  | 1:A:425:ILE:HD11 | 0.50     | 1.82        | 18     | 1     |
| 1:A:370:SER:O    | 1:A:371:PHE:CB   | 0.50     | 2.58        | 6      | 2     |
| 1:A:438:LYS:CG   | 1:A:438:LYS:O    | 0.50     | 2.60        | 15     | 3     |
| 1:A:338:ILE:HG13 | 1:A:385:PHE:CD2  | 0.50     | 2.42        | 20     | 1     |
| 1:A:352:TYR:HD2  | 1:A:368:ILE:HG23 | 0.50     | 1.66        | 4      | 2     |
| 1:A:288:PHE:CE2  | 1:A:443:PHE:CZ   | 0.50     | 3.00        | 9      | 1     |
| 1:A:329:PRO:O    | 1:A:332:ILE:CD1  | 0.50     | 2.60        | 12     | 1     |
| 1:A:384:VAL:CG1  | 1:A:432:VAL:HG13 | 0.50     | 2.36        | 16     | 1     |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:HZ3  | 0.50     | 1.58        | 17     | 1     |
| 1:A:443:PHE:CE2  | 1:A:448:GLN:HG2  | 0.50     | 2.42        | 20     | 1     |
| 1:A:298:ILE:HD12 | 1:A:310:VAL:HB   | 0.50     | 1.84        | 18     | 1     |
| 1:A:443:PHE:CD1  | 1:A:464:SER:HA   | 0.50     | 2.42        | 15     | 1     |
| 1:A:432:VAL:CG2  | 1:A:433:PHE:N    | 0.50     | 2.75        | 13     | 1     |
| 1:A:433:PHE:CE2  | 1:A:441:TYR:CB   | 0.50     | 2.94        | 3      | 2     |
| 1:A:292:THR:HG21 | 1:A:337:GLU:OE2  | 0.50     | 2.07        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:288:PHE:CE1  | 1:A:443:PHE:CE2  | 0.49     | 3.00        | 18     | 1     |
| 1:A:374:PRO:HB3  | 1:A:401:TRP:CZ2  | 0.49     | 2.42        | 13     | 1     |
| 1:A:429:ILE:CD1  | 1:A:431:ALA:O    | 0.49     | 2.60        | 7      | 1     |
| 1:A:285:ASN:ND2  | 1:A:285:ASN:N    | 0.49     | 2.58        | 9      | 2     |
| 1:A:377:VAL:CG1  | 1:A:378:LYS:N    | 0.49     | 2.74        | 6      | 2     |
| 1:A:422:PHE:CE2  | 1:A:456:GLN:HG2  | 0.49     | 2.43        | 13     | 1     |
| 1:A:304:ARG:HG2  | 1:A:305:PHE:CD2  | 0.49     | 2.42        | 11     | 1     |
| 1:A:336:TYR:CZ   | 1:A:345:PHE:HB2  | 0.49     | 2.42        | 9      | 2     |
| 1:A:433:PHE:CD1  | 1:A:433:PHE:C    | 0.49     | 2.84        | 15     | 1     |
| 1:A:443:PHE:CD1  | 1:A:448:GLN:CG   | 0.49     | 2.95        | 15     | 1     |
| 1:A:298:ILE:CG2  | 1:A:300:PHE:CZ   | 0.49     | 2.95        | 9      | 1     |
| 1:A:352:TYR:CZ   | 1:A:366:LYS:HB2  | 0.49     | 2.42        | 5      | 2     |
| 1:A:350:ASP:OD1  | 1:A:368:ILE:HD11 | 0.49     | 2.08        | 1      | 1     |
| 1:A:281:LEU:HD11 | 1:A:307:TRP:CH2  | 0.49     | 2.42        | 11     | 1     |
| 1:A:309:LYS:CB   | 1:A:316:THR:HG22 | 0.49     | 2.37        | 10     | 1     |
| 1:A:310:VAL:HG13 | 1:A:311:SER:OG   | 0.49     | 2.07        | 16     | 1     |
| 1:A:310:VAL:HG22 | 1:A:311:SER:N    | 0.49     | 2.23        | 15     | 8     |
| 1:A:431:ALA:O    | 1:A:432:VAL:HG13 | 0.49     | 2.08        | 14     | 1     |
| 1:A:395:PHE:CD1  | 1:A:418:ILE:HG12 | 0.49     | 2.43        | 9      | 1     |
| 1:A:352:TYR:N    | 1:A:352:TYR:CD1  | 0.49     | 2.80        | 5      | 2     |
| 1:A:302:LYS:O    | 1:A:305:PHE:O    | 0.49     | 2.30        | 20     | 2     |
| 1:A:425:ILE:HG22 | 1:A:442:PHE:CE1  | 0.49     | 2.43        | 20     | 2     |
| 1:A:286:LEU:HD23 | 1:A:286:LEU:C    | 0.49     | 2.27        | 1      | 1     |
| 1:A:294:VAL:HG12 | 1:A:294:VAL:O    | 0.49     | 2.07        | 9      | 1     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CG   | 0.49     | 2.96        | 17     | 1     |
| 1:A:374:PRO:CB   | 1:A:401:TRP:CZ2  | 0.49     | 2.96        | 20     | 1     |
| 1:A:374:PRO:HB2  | 1:A:401:TRP:CZ2  | 0.49     | 2.42        | 20     | 1     |
| 1:A:429:ILE:HG12 | 1:A:442:PHE:CD1  | 0.49     | 2.42        | 13     | 2     |
| 1:A:458:ILE:HG22 | 1:A:458:ILE:O    | 0.49     | 2.07        | 11     | 1     |
| 1:A:436:LYS:HG2  | 1:A:441:TYR:CE1  | 0.49     | 2.43        | 13     | 1     |
| 1:A:355:ILE:O    | 1:A:355:ILE:HG22 | 0.49     | 2.07        | 7      | 1     |
| 1:A:421:ASN:OD1  | 1:A:422:PHE:CD2  | 0.49     | 2.66        | 7      | 2     |
| 1:A:345:PHE:CE2  | 1:A:352:TYR:CE1  | 0.49     | 3.01        | 11     | 1     |
| 1:A:462:LEU:CD1  | 1:A:466:SER:OG   | 0.49     | 2.61        | 2      | 1     |
| 1:A:288:PHE:CE2  | 1:A:300:PHE:CE1  | 0.49     | 3.01        | 4      | 2     |
| 1:A:398:ASN:O    | 1:A:417:LEU:CD1  | 0.49     | 2.61        | 14     | 2     |
| 1:A:318:VAL:HG12 | 1:A:318:VAL:O    | 0.49     | 2.08        | 7      | 1     |
| 1:A:462:LEU:HD11 | 1:A:466:SER:HB2  | 0.49     | 1.83        | 2      | 1     |
| 1:A:422:PHE:CE2  | 1:A:451:TYR:CD1  | 0.49     | 3.01        | 1      | 1     |
| 1:A:432:VAL:HG23 | 1:A:442:PHE:CD1  | 0.49     | 2.43        | 1      | 1     |
| 1:A:393:TYR:CE2  | 1:A:400:TYR:OH   | 0.49     | 2.58        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:441:TYR:CZ   | 1:A:450:GLU:CG   | 0.49     | 2.96        | 5      | 2     |
| 1:A:286:LEU:HD13 | 1:A:287:SER:N    | 0.49     | 2.22        | 9      | 1     |
| 1:A:441:TYR:CE1  | 1:A:450:GLU:HG3  | 0.48     | 2.43        | 14     | 7     |
| 1:A:449:PHE:HB2  | 1:A:451:TYR:CE1  | 0.48     | 2.43        | 13     | 1     |
| 1:A:373:PHE:CZ   | 1:A:377:VAL:O    | 0.48     | 2.66        | 14     | 1     |
| 1:A:428:LYS:O    | 1:A:444:GLN:CG   | 0.48     | 2.61        | 9      | 1     |
| 1:A:387:PRO:O    | 1:A:390:TYR:CE1  | 0.48     | 2.66        | 11     | 1     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:CG   | 0.48     | 2.96        | 16     | 2     |
| 1:A:288:PHE:CZ   | 1:A:443:PHE:CE2  | 0.48     | 3.01        | 18     | 1     |
| 1:A:373:PHE:HA   | 1:A:377:VAL:HG12 | 0.48     | 1.85        | 1      | 1     |
| 1:A:453:PHE:O    | 1:A:453:PHE:CD1  | 0.48     | 2.67        | 13     | 2     |
| 1:A:441:TYR:CZ   | 1:A:450:GLU:HG2  | 0.48     | 2.43        | 13     | 1     |
| 1:A:431:ALA:O    | 1:A:432:VAL:CG1  | 0.48     | 2.61        | 14     | 1     |
| 1:A:291:VAL:HG23 | 1:A:433:PHE:HB3  | 0.48     | 1.86        | 19     | 1     |
| 1:A:367:SER:HB3  | 1:A:369:HIS:CE1  | 0.48     | 2.43        | 19     | 1     |
| 1:A:374:PRO:HD2  | 1:A:377:VAL:HG21 | 0.48     | 1.85        | 12     | 1     |
| 1:A:355:ILE:N    | 1:A:355:ILE:CD1  | 0.48     | 2.77        | 11     | 1     |
| 1:A:306:PHE:HB3  | 1:A:321:ILE:HD11 | 0.48     | 1.84        | 19     | 1     |
| 1:A:373:PHE:CZ   | 1:A:375:ASN:HA   | 0.48     | 2.44        | 10     | 2     |
| 1:A:338:ILE:HD11 | 1:A:385:PHE:CB   | 0.48     | 2.38        | 20     | 1     |
| 1:A:443:PHE:CE1  | 1:A:464:SER:HB2  | 0.48     | 2.44        | 18     | 1     |
| 1:A:364:TYR:CE1  | 1:A:366:LYS:CE   | 0.48     | 2.97        | 4      | 3     |
| 1:A:441:TYR:CZ   | 1:A:450:GLU:OE1  | 0.48     | 2.66        | 17     | 1     |
| 1:A:315:LYS:O    | 1:A:316:THR:CG2  | 0.48     | 2.62        | 3      | 1     |
| 1:A:433:PHE:CZ   | 1:A:441:TYR:HB3  | 0.48     | 2.43        | 5      | 1     |
| 1:A:303:ASP:O    | 1:A:305:PHE:N    | 0.48     | 2.44        | 16     | 2     |
| 1:A:336:TYR:O    | 1:A:336:TYR:CD2  | 0.48     | 2.67        | 5      | 2     |
| 1:A:374:PRO:HG2  | 1:A:401:TRP:CH2  | 0.48     | 2.42        | 1      | 1     |
| 1:A:371:PHE:CD2  | 1:A:371:PHE:O    | 0.48     | 2.66        | 15     | 1     |
| 1:A:467:TRP:C    | 1:A:468:PHE:CD2  | 0.48     | 2.87        | 7      | 2     |
| 1:A:307:TRP:CZ3  | 1:A:468:PHE:CZ   | 0.48     | 3.02        | 6      | 2     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CE1  | 0.48     | 3.01        | 16     | 1     |
| 1:A:421:ASN:OD1  | 1:A:422:PHE:CZ   | 0.48     | 2.67        | 4      | 1     |
| 1:A:440:TYR:CD1  | 1:A:440:TYR:C    | 0.48     | 2.84        | 15     | 1     |
| 1:A:449:PHE:CE2  | 1:A:461:THR:HG21 | 0.48     | 2.43        | 20     | 1     |
| 1:A:412:PRO:O    | 1:A:414:TYR:N    | 0.48     | 2.46        | 19     | 1     |
| 1:A:291:VAL:CG2  | 1:A:300:PHE:CE2  | 0.48     | 2.94        | 16     | 1     |
| 1:A:429:ILE:HD12 | 1:A:444:GLN:OE1  | 0.48     | 2.08        | 16     | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CE2  | 0.48     | 2.44        | 6      | 2     |
| 1:A:449:PHE:CZ   | 1:A:461:THR:CG2  | 0.48     | 2.96        | 20     | 1     |
| 1:A:462:LEU:HD13 | 1:A:462:LEU:N    | 0.48     | 2.24        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:298:ILE:O    | 1:A:308:LEU:CD2  | 0.48     | 2.61        | 9      | 1     |
| 1:A:344:VAL:HG12 | 1:A:346:LEU:HD22 | 0.48     | 1.86        | 10     | 1     |
| 1:A:297:LYS:CA   | 1:A:310:VAL:HG11 | 0.48     | 2.36        | 5      | 1     |
| 1:A:281:LEU:HB3  | 1:A:468:PHE:CZ   | 0.48     | 2.44        | 2      | 1     |
| 1:A:354:LEU:HD22 | 1:A:354:LEU:O    | 0.48     | 2.09        | 15     | 1     |
| 1:A:374:PRO:O    | 1:A:376:PHE:N    | 0.48     | 2.47        | 13     | 1     |
| 1:A:336:TYR:CG   | 1:A:337:GLU:N    | 0.48     | 2.81        | 19     | 2     |
| 1:A:301:PHE:CD1  | 1:A:301:PHE:N    | 0.48     | 2.82        | 9      | 2     |
| 1:A:327:THR:CG2  | 1:A:327:THR:O    | 0.47     | 2.62        | 2      | 4     |
| 1:A:422:PHE:HB2  | 1:A:425:ILE:HD12 | 0.47     | 1.86        | 2      | 1     |
| 1:A:285:ASN:HD22 | 1:A:285:ASN:N    | 0.47     | 2.07        | 14     | 1     |
| 1:A:295:GLY:O    | 1:A:296:ASN:CB   | 0.47     | 2.62        | 14     | 2     |
| 1:A:419:THR:O    | 1:A:423:GLN:N    | 0.47     | 2.47        | 19     | 2     |
| 1:A:455:LEU:O    | 1:A:456:GLN:CB   | 0.47     | 2.62        | 5      | 2     |
| 1:A:354:LEU:HD23 | 1:A:361:GLU:CG   | 0.47     | 2.38        | 16     | 1     |
| 1:A:374:PRO:HD2  | 1:A:377:VAL:HG12 | 0.47     | 1.85        | 16     | 1     |
| 1:A:281:LEU:CD1  | 1:A:307:TRP:CZ3  | 0.47     | 2.83        | 17     | 1     |
| 1:A:354:LEU:CD1  | 1:A:354:LEU:C    | 0.47     | 2.81        | 17     | 1     |
| 1:A:310:VAL:HG13 | 1:A:312:GLU:N    | 0.47     | 2.24        | 11     | 1     |
| 1:A:291:VAL:HG12 | 1:A:431:ALA:HB1  | 0.47     | 1.86        | 18     | 1     |
| 1:A:338:ILE:CG2  | 1:A:339:GLU:N    | 0.47     | 2.77        | 18     | 1     |
| 1:A:288:PHE:CD1  | 1:A:443:PHE:CE2  | 0.47     | 3.01        | 18     | 1     |
| 1:A:328:LEU:CD1  | 1:A:346:LEU:HD12 | 0.47     | 2.39        | 4      | 1     |
| 1:A:368:ILE:O    | 1:A:372:GLY:N    | 0.47     | 2.47        | 6      | 2     |
| 1:A:440:TYR:HB3  | 1:A:442:PHE:CE1  | 0.47     | 2.43        | 5      | 1     |
| 1:A:434:TYR:CD1  | 1:A:439:TYR:O    | 0.47     | 2.67        | 2      | 1     |
| 1:A:288:PHE:CD2  | 1:A:443:PHE:CE2  | 0.47     | 3.03        | 18     | 1     |
| 1:A:418:ILE:CG2  | 1:A:425:ILE:HD11 | 0.47     | 2.39        | 14     | 2     |
| 1:A:311:SER:O    | 1:A:312:GLU:C    | 0.47     | 2.51        | 17     | 4     |
| 1:A:364:TYR:CD1  | 1:A:365:PRO:N    | 0.47     | 2.83        | 12     | 1     |
| 1:A:352:TYR:CE2  | 1:A:366:LYS:HB2  | 0.47     | 2.45        | 12     | 1     |
| 1:A:348:LYS:O    | 1:A:350:ASP:N    | 0.47     | 2.47        | 10     | 1     |
| 1:A:307:TRP:CE2  | 1:A:318:VAL:HG12 | 0.47     | 2.44        | 5      | 1     |
| 1:A:368:ILE:CD1  | 1:A:377:VAL:HG13 | 0.47     | 2.30        | 2      | 1     |
| 1:A:307:TRP:NE1  | 1:A:318:VAL:HG22 | 0.47     | 2.24        | 18     | 1     |
| 1:A:407:ARG:O    | 1:A:408:GLN:CB   | 0.47     | 2.62        | 12     | 9     |
| 1:A:307:TRP:CH2  | 1:A:318:VAL:HG13 | 0.47     | 2.45        | 8      | 1     |
| 1:A:344:VAL:O    | 1:A:345:PHE:CD1  | 0.47     | 2.68        | 9      | 1     |
| 1:A:352:TYR:CD2  | 1:A:366:LYS:HB3  | 0.47     | 2.44        | 11     | 1     |
| 1:A:346:LEU:N    | 1:A:346:LEU:CD2  | 0.47     | 2.74        | 10     | 1     |
| 1:A:298:ILE:HD12 | 1:A:300:PHE:HZ   | 0.47     | 1.69        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:414:TYR:CE2  | 1:A:416:LYS:HG3  | 0.47     | 2.45        | 4      | 11    |
| 1:A:316:THR:HG21 | 1:A:468:PHE:CD1  | 0.47     | 2.43        | 11     | 3     |
| 1:A:301:PHE:CD2  | 1:A:332:ILE:HB   | 0.47     | 2.45        | 8      | 1     |
| 1:A:305:PHE:CD2  | 1:A:318:VAL:CG1  | 0.47     | 2.98        | 6      | 1     |
| 1:A:315:LYS:HG2  | 1:A:468:PHE:CE2  | 0.47     | 2.45        | 3      | 1     |
| 1:A:369:HIS:CE1  | 1:A:373:PHE:CZ   | 0.47     | 3.02        | 16     | 1     |
| 1:A:372:GLY:O    | 1:A:374:PRO:N    | 0.47     | 2.47        | 11     | 6     |
| 1:A:293:THR:HG21 | 1:A:435:SER:HB2  | 0.47     | 1.86        | 3      | 2     |
| 1:A:352:TYR:CZ   | 1:A:366:LYS:HB3  | 0.47     | 2.45        | 18     | 8     |
| 1:A:306:PHE:CZ   | 1:A:319:ASN:HB2  | 0.47     | 2.44        | 10     | 4     |
| 1:A:300:PHE:C    | 1:A:300:PHE:CD1  | 0.47     | 2.87        | 18     | 1     |
| 1:A:343:GLN:NE2  | 1:A:354:LEU:HD11 | 0.47     | 2.25        | 14     | 1     |
| 1:A:459:THR:OG1  | 1:A:460:LYS:N    | 0.47     | 2.47        | 7      | 1     |
| 1:A:418:ILE:H    | 1:A:418:ILE:HD12 | 0.47     | 1.68        | 8      | 2     |
| 1:A:293:THR:HG21 | 1:A:435:SER:OG   | 0.47     | 2.09        | 9      | 1     |
| 1:A:286:LEU:HD23 | 1:A:287:SER:H    | 0.47     | 1.69        | 11     | 1     |
| 1:A:347:PHE:CE2  | 1:A:352:TYR:CE1  | 0.47     | 3.02        | 6      | 1     |
| 1:A:461:THR:O    | 1:A:461:THR:CG2  | 0.47     | 2.60        | 6      | 1     |
| 1:A:347:PHE:CE2  | 1:A:380:ILE:HB   | 0.47     | 2.45        | 5      | 1     |
| 1:A:448:GLN:O    | 1:A:462:LEU:CD2  | 0.47     | 2.63        | 5      | 1     |
| 1:A:339:GLU:O    | 1:A:342:ASN:N    | 0.47     | 2.48        | 18     | 1     |
| 1:A:460:LYS:HE2  | 1:A:462:LEU:HD22 | 0.47     | 1.86        | 18     | 1     |
| 1:A:418:ILE:HG22 | 1:A:425:ILE:CD1  | 0.47     | 2.39        | 14     | 1     |
| 1:A:352:TYR:O    | 1:A:352:TYR:CG   | 0.47     | 2.67        | 11     | 1     |
| 1:A:448:GLN:CB   | 1:A:462:LEU:CD2  | 0.47     | 2.92        | 16     | 1     |
| 1:A:434:TYR:CE1  | 1:A:439:TYR:O    | 0.47     | 2.68        | 2      | 1     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HD3  | 0.47     | 2.44        | 6      | 2     |
| 1:A:375:ASN:O    | 1:A:376:PHE:C    | 0.47     | 2.54        | 13     | 1     |
| 1:A:400:TYR:CE1  | 1:A:402:ARG:HG3  | 0.47     | 2.45        | 7      | 1     |
| 1:A:341:ARG:O    | 1:A:342:ASN:CB   | 0.47     | 2.63        | 19     | 2     |
| 1:A:354:LEU:HD22 | 1:A:354:LEU:C    | 0.47     | 2.30        | 15     | 1     |
| 1:A:395:PHE:HE2  | 1:A:432:VAL:HG21 | 0.47     | 1.69        | 9      | 2     |
| 1:A:300:PHE:O    | 1:A:307:TRP:CE3  | 0.47     | 2.68        | 8      | 1     |
| 1:A:439:TYR:CE1  | 1:A:452:ASP:HB2  | 0.47     | 2.44        | 10     | 1     |
| 1:A:433:PHE:CD1  | 1:A:433:PHE:N    | 0.46     | 2.83        | 5      | 3     |
| 1:A:301:PHE:CE1  | 1:A:321:ILE:HG12 | 0.46     | 2.45        | 2      | 1     |
| 1:A:418:ILE:CD1  | 1:A:427:PRO:O    | 0.46     | 2.63        | 17     | 3     |
| 1:A:292:THR:HB   | 1:A:335:ALA:HB1  | 0.46     | 1.86        | 7      | 2     |
| 1:A:307:TRP:CE2  | 1:A:316:THR:CB   | 0.46     | 2.98        | 14     | 1     |
| 1:A:301:PHE:CD2  | 1:A:332:ILE:HG12 | 0.46     | 2.45        | 7      | 1     |
| 1:A:298:ILE:CG2  | 1:A:300:PHE:CE1  | 0.46     | 2.98        | 9      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:403:TYR:CE2  | 1:A:405:GLU:OE2  | 0.46     | 2.67        | 6      | 1     |
| 1:A:429:ILE:CD1  | 1:A:444:GLN:OE1  | 0.46     | 2.64        | 16     | 1     |
| 1:A:301:PHE:CZ   | 1:A:332:ILE:HD13 | 0.46     | 2.45        | 1      | 1     |
| 1:A:418:ILE:O    | 1:A:420:LYS:N    | 0.46     | 2.48        | 1      | 4     |
| 1:A:306:PHE:CE2  | 1:A:319:ASN:HB3  | 0.46     | 2.45        | 14     | 1     |
| 1:A:451:TYR:CE1  | 1:A:456:GLN:HA   | 0.46     | 2.45        | 6      | 1     |
| 1:A:460:LYS:O    | 1:A:461:THR:HG23 | 0.46     | 2.10        | 3      | 1     |
| 1:A:430:ASP:CB   | 1:A:443:PHE:O    | 0.46     | 2.64        | 2      | 5     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HE3  | 0.46     | 2.45        | 8      | 3     |
| 1:A:433:PHE:CE1  | 1:A:441:TYR:O    | 0.46     | 2.69        | 9      | 1     |
| 1:A:436:LYS:HD3  | 1:A:441:TYR:CE1  | 0.46     | 2.46        | 10     | 2     |
| 1:A:433:PHE:N    | 1:A:433:PHE:CD1  | 0.46     | 2.84        | 1      | 2     |
| 1:A:288:PHE:CG   | 1:A:443:PHE:CE2  | 0.46     | 3.03        | 18     | 1     |
| 1:A:432:VAL:HG23 | 1:A:440:TYR:CD1  | 0.46     | 2.44        | 15     | 1     |
| 1:A:448:GLN:CB   | 1:A:462:LEU:HD21 | 0.46     | 2.40        | 14     | 1     |
| 1:A:391:ARG:CZ   | 1:A:404:ASP:OD1  | 0.46     | 2.63        | 9      | 1     |
| 1:A:307:TRP:CE3  | 1:A:318:VAL:HB   | 0.46     | 2.46        | 17     | 1     |
| 1:A:308:LEU:C    | 1:A:308:LEU:CD2  | 0.46     | 2.84        | 20     | 1     |
| 1:A:352:TYR:CZ   | 1:A:366:LYS:CB   | 0.46     | 2.99        | 18     | 2     |
| 1:A:356:SER:O    | 1:A:358:LEU:N    | 0.46     | 2.49        | 6      | 3     |
| 1:A:460:LYS:C    | 1:A:461:THR:CG2  | 0.46     | 2.84        | 13     | 1     |
| 1:A:422:PHE:HB3  | 1:A:451:TYR:CE2  | 0.46     | 2.46        | 8      | 2     |
| 1:A:311:SER:OG   | 1:A:312:GLU:N    | 0.46     | 2.49        | 9      | 1     |
| 1:A:388:ARG:O    | 1:A:390:TYR:CE2  | 0.46     | 2.68        | 11     | 1     |
| 1:A:299:PHE:HB3  | 1:A:301:PHE:CE1  | 0.46     | 2.45        | 3      | 1     |
| 1:A:432:VAL:HB   | 1:A:442:PHE:CD1  | 0.46     | 2.45        | 13     | 3     |
| 1:A:430:ASP:N    | 1:A:430:ASP:OD1  | 0.46     | 2.49        | 6      | 2     |
| 1:A:329:PRO:HG3  | 1:A:353:TRP:CZ3  | 0.46     | 2.46        | 1      | 1     |
| 1:A:380:ILE:HG22 | 1:A:381:ASP:N    | 0.46     | 2.26        | 12     | 3     |
| 1:A:334:ALA:HB1  | 1:A:382:ALA:HA   | 0.46     | 1.88        | 4      | 1     |
| 1:A:455:LEU:CD2  | 1:A:455:LEU:N    | 0.46     | 2.78        | 14     | 1     |
| 1:A:382:ALA:HB3  | 1:A:395:PHE:HD2  | 0.46     | 1.70        | 12     | 1     |
| 1:A:377:VAL:HG12 | 1:A:378:LYS:N    | 0.46     | 2.24        | 10     | 1     |
| 1:A:445:GLY:O    | 1:A:447:ASN:ND2  | 0.46     | 2.49        | 16     | 3     |
| 1:A:393:TYR:C    | 1:A:394:PHE:CD1  | 0.46     | 2.89        | 1      | 1     |
| 1:A:302:LYS:O    | 1:A:304:ARG:N    | 0.46     | 2.49        | 6      | 3     |
| 1:A:352:TYR:CD2  | 1:A:368:ILE:HG23 | 0.46     | 2.45        | 4      | 1     |
| 1:A:364:TYR:CG   | 1:A:366:LYS:HE3  | 0.46     | 2.46        | 7      | 4     |
| 1:A:299:PHE:HB3  | 1:A:301:PHE:CZ   | 0.46     | 2.46        | 3      | 2     |
| 1:A:325:TRP:CG   | 1:A:328:LEU:CB   | 0.46     | 2.99        | 10     | 1     |
| 1:A:371:PHE:O    | 1:A:371:PHE:CG   | 0.46     | 2.69        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:429:ILE:CD1  | 1:A:442:PHE:CD2  | 0.46     | 2.98        | 20     | 1     |
| 1:A:336:TYR:CE1  | 1:A:345:PHE:CG   | 0.46     | 3.04        | 2      | 1     |
| 1:A:419:THR:HG23 | 1:A:420:LYS:N    | 0.46     | 2.26        | 18     | 2     |
| 1:A:385:PHE:C    | 1:A:385:PHE:CD1  | 0.46     | 2.89        | 1      | 1     |
| 1:A:293:THR:O    | 1:A:337:GLU:CG   | 0.46     | 2.63        | 13     | 1     |
| 1:A:293:THR:HG21 | 1:A:435:SER:HA   | 0.46     | 1.86        | 14     | 1     |
| 1:A:437:ASN:O    | 1:A:439:TYR:CD2  | 0.46     | 2.69        | 17     | 2     |
| 1:A:386:ASN:ND2  | 1:A:393:TYR:CE1  | 0.46     | 2.83        | 17     | 2     |
| 1:A:449:PHE:CD1  | 1:A:461:THR:HG23 | 0.46     | 2.46        | 17     | 1     |
| 1:A:293:THR:HG21 | 1:A:435:SER:HB3  | 0.46     | 1.87        | 20     | 1     |
| 1:A:441:TYR:CD1  | 1:A:450:GLU:HG3  | 0.46     | 2.46        | 6      | 1     |
| 1:A:447:ASN:OD1  | 1:A:449:PHE:CE2  | 0.46     | 2.69        | 2      | 1     |
| 1:A:318:VAL:HG13 | 1:A:318:VAL:O    | 0.46     | 2.11        | 15     | 1     |
| 1:A:338:ILE:CG2  | 1:A:338:ILE:O    | 0.46     | 2.64        | 13     | 1     |
| 1:A:352:TYR:CE1  | 1:A:366:LYS:HB3  | 0.46     | 2.47        | 9      | 2     |
| 1:A:321:ILE:O    | 1:A:324:LEU:N    | 0.46     | 2.47        | 10     | 5     |
| 1:A:463:LYS:O    | 1:A:466:SER:N    | 0.46     | 2.49        | 17     | 1     |
| 1:A:372:GLY:C    | 1:A:373:PHE:CD1  | 0.46     | 2.89        | 20     | 1     |
| 1:A:431:ALA:HB3  | 1:A:443:PHE:HB2  | 0.46     | 1.87        | 3      | 1     |
| 1:A:392:THR:HG22 | 1:A:393:TYR:H    | 0.46     | 1.70        | 19     | 1     |
| 1:A:397:ASP:OD1  | 1:A:397:ASP:N    | 0.46     | 2.49        | 19     | 1     |
| 1:A:299:PHE:CD1  | 1:A:308:LEU:HD21 | 0.45     | 2.47        | 2      | 1     |
| 1:A:298:ILE:CD1  | 1:A:300:PHE:CZ   | 0.45     | 2.90        | 13     | 1     |
| 1:A:432:VAL:HG12 | 1:A:442:PHE:HD1  | 0.45     | 1.71        | 9      | 1     |
| 1:A:345:PHE:O    | 1:A:346:LEU:HD22 | 0.45     | 2.11        | 5      | 2     |
| 1:A:441:TYR:CE2  | 1:A:450:GLU:HG3  | 0.45     | 2.47        | 5      | 1     |
| 1:A:433:PHE:CE2  | 1:A:435:SER:HB3  | 0.45     | 2.46        | 19     | 1     |
| 1:A:393:TYR:N    | 1:A:393:TYR:CD1  | 0.45     | 2.84        | 1      | 1     |
| 1:A:403:TYR:CD2  | 1:A:410:MET:HB3  | 0.45     | 2.46        | 4      | 1     |
| 1:A:391:ARG:NH1  | 1:A:404:ASP:OD2  | 0.45     | 2.50        | 14     | 1     |
| 1:A:387:PRO:HG2  | 1:A:434:TYR:CZ   | 0.45     | 2.47        | 7      | 1     |
| 1:A:321:ILE:HG22 | 1:A:322:SER:N    | 0.45     | 2.27        | 20     | 3     |
| 1:A:354:LEU:O    | 1:A:354:LEU:HD13 | 0.45     | 2.11        | 11     | 1     |
| 1:A:338:ILE:CD1  | 1:A:340:ALA:HB3  | 0.45     | 2.40        | 3      | 1     |
| 1:A:354:LEU:C    | 1:A:354:LEU:CD1  | 0.45     | 2.78        | 18     | 2     |
| 1:A:403:TYR:CE2  | 1:A:410:MET:HB3  | 0.45     | 2.45        | 10     | 2     |
| 1:A:467:TRP:O    | 1:A:468:PHE:C    | 0.45     | 2.55        | 10     | 2     |
| 1:A:281:LEU:HD21 | 1:A:307:TRP:CE3  | 0.45     | 2.46        | 17     | 1     |
| 1:A:395:PHE:CE2  | 1:A:432:VAL:HG11 | 0.45     | 2.46        | 17     | 1     |
| 1:A:293:THR:HG22 | 1:A:433:PHE:CE2  | 0.45     | 2.46        | 6      | 1     |
| 1:A:307:TRP:HE1  | 1:A:318:VAL:HG22 | 0.45     | 1.72        | 18     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:291:VAL:HG11 | 1:A:442:PHE:HZ   | 0.45     | 1.71        | 15     | 1     |
| 1:A:307:TRP:CZ3  | 1:A:318:VAL:HB   | 0.45     | 2.47        | 11     | 2     |
| 1:A:468:PHE:CD1  | 1:A:470:CYS:HB2  | 0.45     | 2.47        | 20     | 2     |
| 1:A:281:LEU:HA   | 1:A:286:LEU:HD12 | 0.45     | 1.89        | 17     | 1     |
| 1:A:297:LYS:HG2  | 1:A:299:PHE:CZ   | 0.45     | 2.47        | 19     | 1     |
| 1:A:302:LYS:N    | 1:A:305:PHE:O    | 0.45     | 2.49        | 1      | 4     |
| 1:A:400:TYR:CE2  | 1:A:418:ILE:HA   | 0.45     | 2.46        | 13     | 1     |
| 1:A:436:LYS:HE3  | 1:A:441:TYR:CE2  | 0.45     | 2.46        | 8      | 1     |
| 1:A:336:TYR:OH   | 1:A:345:PHE:CG   | 0.45     | 2.64        | 9      | 1     |
| 1:A:433:PHE:CE2  | 1:A:443:PHE:CE1  | 0.45     | 3.05        | 12     | 1     |
| 1:A:448:GLN:HB3  | 1:A:462:LEU:HD21 | 0.45     | 1.87        | 11     | 1     |
| 1:A:373:PHE:CD1  | 1:A:377:VAL:HG21 | 0.45     | 2.46        | 6      | 1     |
| 1:A:308:LEU:HD21 | 1:A:313:ARG:CZ   | 0.45     | 2.41        | 16     | 1     |
| 1:A:360:PRO:O    | 1:A:361:GLU:C    | 0.45     | 2.54        | 16     | 4     |
| 1:A:463:LYS:O    | 1:A:466:SER:CB   | 0.45     | 2.65        | 16     | 1     |
| 1:A:288:PHE:CD2  | 1:A:443:PHE:CD1  | 0.45     | 3.04        | 7      | 1     |
| 1:A:301:PHE:O    | 1:A:302:LYS:C    | 0.45     | 2.54        | 7      | 1     |
| 1:A:299:PHE:C    | 1:A:300:PHE:CG   | 0.45     | 2.90        | 11     | 1     |
| 1:A:414:TYR:N    | 1:A:415:PRO:CD   | 0.45     | 2.79        | 19     | 1     |
| 1:A:441:TYR:CD2  | 1:A:448:GLN:OE1  | 0.45     | 2.69        | 16     | 1     |
| 1:A:462:LEU:CD2  | 1:A:466:SER:OG   | 0.45     | 2.65        | 2      | 1     |
| 1:A:418:ILE:O    | 1:A:419:THR:C    | 0.45     | 2.53        | 14     | 5     |
| 1:A:393:TYR:CD2  | 1:A:400:TYR:CE1  | 0.45     | 3.05        | 4      | 2     |
| 1:A:296:ASN:ND2  | 1:A:296:ASN:O    | 0.45     | 2.50        | 20     | 2     |
| 1:A:298:ILE:C    | 1:A:299:PHE:CD1  | 0.45     | 2.90        | 11     | 2     |
| 1:A:294:VAL:O    | 1:A:296:ASN:N    | 0.45     | 2.49        | 12     | 2     |
| 1:A:307:TRP:CE3  | 1:A:317:SER:O    | 0.45     | 2.69        | 11     | 1     |
| 1:A:315:LYS:C    | 1:A:316:THR:HG23 | 0.45     | 2.32        | 3      | 1     |
| 1:A:344:VAL:N    | 1:A:355:ILE:O    | 0.45     | 2.49        | 3      | 1     |
| 1:A:418:ILE:O    | 1:A:421:ASN:N    | 0.45     | 2.50        | 16     | 1     |
| 1:A:463:LYS:O    | 1:A:464:SER:C    | 0.45     | 2.55        | 17     | 2     |
| 1:A:447:ASN:ND2  | 1:A:447:ASN:N    | 0.45     | 2.64        | 20     | 1     |
| 1:A:433:PHE:O    | 1:A:441:TYR:N    | 0.45     | 2.49        | 6      | 1     |
| 1:A:286:LEU:HD23 | 1:A:287:SER:N    | 0.45     | 2.27        | 20     | 1     |
| 1:A:338:ILE:CD1  | 1:A:385:PHE:CD2  | 0.45     | 3.00        | 6      | 1     |
| 1:A:354:LEU:CD1  | 1:A:354:LEU:N    | 0.44     | 2.80        | 15     | 1     |
| 1:A:364:TYR:CZ   | 1:A:366:LYS:HD3  | 0.44     | 2.47        | 15     | 2     |
| 1:A:443:PHE:CZ   | 1:A:448:GLN:NE2  | 0.44     | 2.84        | 9      | 1     |
| 1:A:345:PHE:CE2  | 1:A:354:LEU:HD13 | 0.44     | 2.48        | 12     | 1     |
| 1:A:425:ILE:O    | 1:A:444:GLN:NE2  | 0.44     | 2.49        | 12     | 1     |
| 1:A:328:LEU:HD23 | 1:A:360:PRO:HB3  | 0.44     | 1.90        | 10     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:336:TYR:CE2  | 1:A:338:ILE:CG1  | 0.44     | 3.00        | 10     | 1     |
| 1:A:432:VAL:HG21 | 1:A:442:PHE:CD2  | 0.44     | 2.47        | 5      | 1     |
| 1:A:305:PHE:HB3  | 1:A:307:TRP:CH2  | 0.44     | 2.47        | 18     | 1     |
| 1:A:380:ILE:CG2  | 1:A:381:ASP:N    | 0.44     | 2.81        | 1      | 1     |
| 1:A:428:LYS:O    | 1:A:444:GLN:NE2  | 0.44     | 2.50        | 4      | 1     |
| 1:A:440:TYR:N    | 1:A:440:TYR:CD1  | 0.44     | 2.84        | 7      | 1     |
| 1:A:344:VAL:C    | 1:A:345:PHE:CD1  | 0.44     | 2.91        | 9      | 1     |
| 1:A:425:ILE:HD13 | 1:A:426:GLY:H    | 0.44     | 1.73        | 12     | 1     |
| 1:A:448:GLN:HG2  | 1:A:462:LEU:HD23 | 0.44     | 1.88        | 3      | 1     |
| 1:A:281:LEU:HB2  | 1:A:468:PHE:CE2  | 0.44     | 2.47        | 5      | 1     |
| 1:A:306:PHE:CE2  | 1:A:319:ASN:C    | 0.44     | 2.91        | 2      | 2     |
| 1:A:286:LEU:HD11 | 1:A:307:TRP:CZ3  | 0.44     | 2.47        | 1      | 1     |
| 1:A:373:PHE:CZ   | 1:A:376:PHE:HA   | 0.44     | 2.47        | 1      | 1     |
| 1:A:384:VAL:HG11 | 1:A:432:VAL:HG22 | 0.44     | 1.88        | 4      | 1     |
| 1:A:291:VAL:HG13 | 1:A:300:PHE:CE1  | 0.44     | 2.47        | 9      | 1     |
| 1:A:294:VAL:O    | 1:A:294:VAL:HG12 | 0.44     | 2.11        | 17     | 1     |
| 1:A:303:ASP:O    | 1:A:331:GLY:N    | 0.44     | 2.49        | 11     | 2     |
| 1:A:292:THR:OG1  | 1:A:335:ALA:CB   | 0.44     | 2.66        | 4      | 1     |
| 1:A:467:TRP:C    | 1:A:468:PHE:CG   | 0.44     | 2.90        | 7      | 2     |
| 1:A:356:SER:O    | 1:A:357:ASN:CB   | 0.44     | 2.65        | 17     | 2     |
| 1:A:368:ILE:O    | 1:A:371:PHE:CD1  | 0.44     | 2.69        | 20     | 1     |
| 1:A:320:LEU:H    | 1:A:320:LEU:HD23 | 0.44     | 1.71        | 19     | 1     |
| 1:A:444:GLN:O    | 1:A:447:ASN:ND2  | 0.44     | 2.50        | 3      | 3     |
| 1:A:448:GLN:O    | 1:A:462:LEU:HD23 | 0.44     | 2.12        | 11     | 2     |
| 1:A:449:PHE:CD1  | 1:A:461:THR:HG22 | 0.44     | 2.47        | 14     | 1     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:OG   | 0.44     | 2.12        | 11     | 1     |
| 1:A:325:TRP:CZ3  | 1:A:328:LEU:HD12 | 0.44     | 2.48        | 10     | 1     |
| 1:A:384:VAL:HG23 | 1:A:432:VAL:HG13 | 0.44     | 1.88        | 10     | 1     |
| 1:A:447:ASN:HB3  | 1:A:449:PHE:CD1  | 0.44     | 2.47        | 6      | 1     |
| 1:A:379:LYS:O    | 1:A:396:VAL:HG23 | 0.44     | 2.13        | 5      | 1     |
| 1:A:338:ILE:HD12 | 1:A:385:PHE:CE2  | 0.44     | 2.47        | 6      | 1     |
| 1:A:447:ASN:HB3  | 1:A:449:PHE:CE1  | 0.44     | 2.47        | 6      | 1     |
| 1:A:286:LEU:HD22 | 1:A:307:TRP:CZ3  | 0.44     | 2.48        | 19     | 1     |
| 1:A:312:GLU:O    | 1:A:314:PRO:N    | 0.44     | 2.51        | 7      | 1     |
| 1:A:394:PHE:CD2  | 1:A:403:TYR:CD1  | 0.44     | 3.05        | 10     | 1     |
| 1:A:306:PHE:CB   | 1:A:319:ASN:O    | 0.44     | 2.66        | 6      | 1     |
| 1:A:391:ARG:NH1  | 1:A:411:ASP:OD2  | 0.44     | 2.51        | 3      | 1     |
| 1:A:453:PHE:C    | 1:A:455:LEU:N    | 0.44     | 2.70        | 13     | 2     |
| 1:A:300:PHE:CD1  | 1:A:300:PHE:N    | 0.44     | 2.86        | 7      | 1     |
| 1:A:350:ASP:O    | 1:A:350:ASP:CG   | 0.44     | 2.54        | 9      | 2     |
| 1:A:283:ASP:O    | 1:A:285:ASN:ND2  | 0.44     | 2.50        | 9      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:395:PHE:HE2  | 1:A:432:VAL:HG11 | 0.44     | 1.73        | 17     | 1     |
| 1:A:440:TYR:HB3  | 1:A:442:PHE:CE2  | 0.44     | 2.48        | 10     | 1     |
| 1:A:281:LEU:CB   | 1:A:468:PHE:CD2  | 0.44     | 3.01        | 5      | 1     |
| 1:A:448:GLN:HB3  | 1:A:462:LEU:CD2  | 0.44     | 2.43        | 16     | 1     |
| 1:A:301:PHE:CD1  | 1:A:321:ILE:HD11 | 0.44     | 2.47        | 2      | 1     |
| 1:A:425:ILE:CG1  | 1:A:426:GLY:N    | 0.44     | 2.81        | 1      | 1     |
| 1:A:449:PHE:CD2  | 1:A:461:THR:CG2  | 0.44     | 3.01        | 13     | 1     |
| 1:A:352:TYR:O    | 1:A:352:TYR:CD2  | 0.44     | 2.71        | 9      | 1     |
| 1:A:306:PHE:CD1  | 1:A:319:ASN:O    | 0.44     | 2.70        | 19     | 1     |
| 1:A:455:LEU:O    | 1:A:456:GLN:C    | 0.43     | 2.56        | 15     | 4     |
| 1:A:329:PRO:O    | 1:A:330:SER:CB   | 0.43     | 2.66        | 19     | 2     |
| 1:A:300:PHE:C    | 1:A:301:PHE:CD1  | 0.43     | 2.91        | 9      | 1     |
| 1:A:353:TRP:CD1  | 1:A:364:TYR:CD1  | 0.43     | 3.06        | 12     | 1     |
| 1:A:350:ASP:OD1  | 1:A:369:HIS:ND1  | 0.43     | 2.50        | 11     | 1     |
| 1:A:442:PHE:N    | 1:A:442:PHE:CD1  | 0.43     | 2.86        | 6      | 1     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CE1  | 0.43     | 3.01        | 6      | 1     |
| 1:A:348:LYS:O    | 1:A:351:LYS:O    | 0.43     | 2.37        | 16     | 11    |
| 1:A:393:TYR:CB   | 1:A:401:TRP:O    | 0.43     | 2.66        | 1      | 1     |
| 1:A:305:PHE:CD2  | 1:A:318:VAL:HG12 | 0.43     | 2.48        | 8      | 1     |
| 1:A:313:ARG:CG   | 1:A:315:LYS:O    | 0.43     | 2.66        | 12     | 1     |
| 1:A:429:ILE:CG1  | 1:A:442:PHE:CD1  | 0.43     | 3.01        | 16     | 1     |
| 1:A:465:ASN:O    | 1:A:468:PHE:N    | 0.43     | 2.51        | 18     | 1     |
| 1:A:310:VAL:CG2  | 1:A:311:SER:N    | 0.43     | 2.81        | 1      | 2     |
| 1:A:358:LEU:CG   | 1:A:358:LEU:O    | 0.43     | 2.66        | 12     | 1     |
| 1:A:440:TYR:CD1  | 1:A:440:TYR:N    | 0.43     | 2.85        | 10     | 1     |
| 1:A:299:PHE:CD2  | 1:A:308:LEU:CD2  | 0.43     | 3.01        | 1      | 2     |
| 1:A:403:TYR:CD1  | 1:A:403:TYR:C    | 0.43     | 2.91        | 1      | 1     |
| 1:A:418:ILE:C    | 1:A:420:LYS:N    | 0.43     | 2.70        | 1      | 5     |
| 1:A:438:LYS:O    | 1:A:438:LYS:CG   | 0.43     | 2.67        | 4      | 2     |
| 1:A:291:VAL:CG2  | 1:A:442:PHE:CZ   | 0.43     | 2.90        | 15     | 1     |
| 1:A:303:ASP:O    | 1:A:304:ARG:CB   | 0.43     | 2.64        | 8      | 1     |
| 1:A:283:ASP:O    | 1:A:465:ASN:ND2  | 0.43     | 2.52        | 12     | 1     |
| 1:A:425:ILE:HG21 | 1:A:442:PHE:CD1  | 0.43     | 2.48        | 17     | 1     |
| 1:A:299:PHE:N    | 1:A:299:PHE:CD1  | 0.43     | 2.86        | 11     | 1     |
| 1:A:419:THR:O    | 1:A:423:GLN:CA   | 0.43     | 2.67        | 11     | 1     |
| 1:A:291:VAL:HG21 | 1:A:300:PHE:CZ   | 0.43     | 2.46        | 16     | 1     |
| 1:A:295:GLY:CA   | 1:A:339:GLU:OE1  | 0.43     | 2.66        | 18     | 1     |
| 1:A:464:SER:O    | 1:A:465:ASN:C    | 0.43     | 2.57        | 18     | 1     |
| 1:A:292:THR:OG1  | 1:A:335:ALA:HB1  | 0.43     | 2.13        | 4      | 1     |
| 1:A:390:TYR:O    | 1:A:405:GLU:N    | 0.43     | 2.50        | 20     | 1     |
| 1:A:435:SER:O    | 1:A:436:LYS:CB   | 0.43     | 2.66        | 20     | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:300:PHE:O    | 1:A:306:PHE:CB   | 0.43     | 2.67        | 16     | 1     |
| 1:A:310:VAL:O    | 1:A:311:SER:O    | 0.43     | 2.36        | 18     | 2     |
| 1:A:384:VAL:CG1  | 1:A:432:VAL:HG12 | 0.43     | 2.41        | 18     | 1     |
| 1:A:425:ILE:HD11 | 1:A:451:TYR:CD1  | 0.43     | 2.49        | 15     | 1     |
| 1:A:424:GLY:C    | 1:A:425:ILE:CG2  | 0.43     | 2.86        | 12     | 1     |
| 1:A:332:ILE:CG2  | 1:A:334:ALA:O    | 0.43     | 2.66        | 4      | 1     |
| 1:A:294:VAL:HG13 | 1:A:294:VAL:O    | 0.43     | 2.14        | 13     | 1     |
| 1:A:304:ARG:N    | 1:A:304:ARG:CD   | 0.43     | 2.81        | 10     | 1     |
| 1:A:438:LYS:CE   | 1:A:438:LYS:HA   | 0.43     | 2.43        | 5      | 1     |
| 1:A:346:LEU:CD2  | 1:A:346:LEU:N    | 0.43     | 2.81        | 2      | 1     |
| 1:A:433:PHE:CE1  | 1:A:441:TYR:CB   | 0.43     | 3.02        | 18     | 1     |
| 1:A:329:PRO:HG3  | 1:A:353:TRP:CE3  | 0.43     | 2.49        | 13     | 1     |
| 1:A:295:GLY:O    | 1:A:296:ASN:OD1  | 0.43     | 2.37        | 14     | 1     |
| 1:A:425:ILE:HD12 | 1:A:442:PHE:CE2  | 0.43     | 2.48        | 14     | 1     |
| 1:A:434:TYR:O    | 1:A:434:TYR:CD2  | 0.43     | 2.71        | 8      | 1     |
| 1:A:293:THR:CG2  | 1:A:435:SER:OG   | 0.43     | 2.67        | 9      | 1     |
| 1:A:364:TYR:CG   | 1:A:365:PRO:CD   | 0.43     | 3.02        | 12     | 1     |
| 1:A:403:TYR:CG   | 1:A:403:TYR:O    | 0.43     | 2.70        | 20     | 1     |
| 1:A:309:LYS:CD   | 1:A:315:LYS:O    | 0.43     | 2.67        | 3      | 1     |
| 1:A:325:TRP:CE3  | 1:A:328:LEU:HG   | 0.43     | 2.48        | 15     | 1     |
| 1:A:442:PHE:CZ   | 1:A:449:PHE:HB2  | 0.43     | 2.49        | 20     | 1     |
| 1:A:296:ASN:O    | 1:A:296:ASN:ND2  | 0.43     | 2.52        | 3      | 1     |
| 1:A:321:ILE:O    | 1:A:322:SER:C    | 0.43     | 2.56        | 5      | 5     |
| 1:A:374:PRO:CG   | 1:A:401:TRP:CH2  | 0.43     | 3.01        | 1      | 1     |
| 1:A:352:TYR:CE1  | 1:A:366:LYS:HB2  | 0.43     | 2.48        | 10     | 1     |
| 1:A:373:PHE:CZ   | 1:A:380:ILE:HG12 | 0.43     | 2.49        | 6      | 1     |
| 1:A:362:PRO:O    | 1:A:363:ASN:CG   | 0.42     | 2.58        | 8      | 2     |
| 1:A:292:THR:CG2  | 1:A:293:THR:N    | 0.42     | 2.81        | 17     | 1     |
| 1:A:430:ASP:N    | 1:A:443:PHE:O    | 0.42     | 2.51        | 10     | 1     |
| 1:A:350:ASP:CG   | 1:A:350:ASP:O    | 0.42     | 2.56        | 6      | 2     |
| 1:A:414:TYR:CZ   | 1:A:416:LYS:HG3  | 0.42     | 2.49        | 5      | 1     |
| 1:A:306:PHE:CD1  | 1:A:321:ILE:HG13 | 0.42     | 2.49        | 19     | 1     |
| 1:A:412:PRO:O    | 1:A:413:GLY:O    | 0.42     | 2.37        | 16     | 4     |
| 1:A:373:PHE:N    | 1:A:374:PRO:HD3  | 0.42     | 2.28        | 20     | 3     |
| 1:A:467:TRP:O    | 1:A:469:GLY:N    | 0.42     | 2.52        | 11     | 1     |
| 1:A:401:TRP:CZ2  | 1:A:412:PRO:HA   | 0.42     | 2.49        | 18     | 1     |
| 1:A:338:ILE:O    | 1:A:341:ARG:N    | 0.42     | 2.52        | 20     | 1     |
| 1:A:442:PHE:HB2  | 1:A:449:PHE:CZ   | 0.42     | 2.49        | 5      | 1     |
| 1:A:438:LYS:HA   | 1:A:438:LYS:CE   | 0.42     | 2.45        | 16     | 1     |
| 1:A:344:VAL:O    | 1:A:355:ILE:HG22 | 0.42     | 2.13        | 4      | 1     |
| 1:A:440:TYR:CD1  | 1:A:441:TYR:N    | 0.42     | 2.87        | 15     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:384:VAL:CG1  | 1:A:385:PHE:N    | 0.42     | 2.82        | 13     | 1     |
| 1:A:336:TYR:CE1  | 1:A:345:PHE:HB2  | 0.42     | 2.49        | 6      | 2     |
| 1:A:306:PHE:CZ   | 1:A:319:ASN:CB   | 0.42     | 3.03        | 12     | 1     |
| 1:A:325:TRP:HB3  | 1:A:328:LEU:CB   | 0.42     | 2.44        | 10     | 1     |
| 1:A:380:ILE:HA   | 1:A:396:VAL:HG22 | 0.42     | 1.90        | 20     | 1     |
| 1:A:322:SER:O    | 1:A:324:LEU:N    | 0.42     | 2.53        | 19     | 1     |
| 1:A:298:ILE:C    | 1:A:298:ILE:HD12 | 0.42     | 2.35        | 4      | 1     |
| 1:A:431:ALA:CB   | 1:A:442:PHE:CE2  | 0.42     | 3.03        | 15     | 1     |
| 1:A:383:ALA:HB1  | 1:A:394:PHE:CE1  | 0.42     | 2.48        | 13     | 1     |
| 1:A:389:PHE:O    | 1:A:390:TYR:CG   | 0.42     | 2.72        | 14     | 2     |
| 1:A:463:LYS:C    | 1:A:465:ASN:N    | 0.42     | 2.72        | 7      | 1     |
| 1:A:322:SER:O    | 1:A:323:SER:C    | 0.42     | 2.57        | 9      | 2     |
| 1:A:451:TYR:CD2  | 1:A:458:ILE:HG13 | 0.42     | 2.50        | 17     | 1     |
| 1:A:399:GLN:CB   | 1:A:416:LYS:O    | 0.42     | 2.67        | 20     | 1     |
| 1:A:337:GLU:CD   | 1:A:338:ILE:N    | 0.42     | 2.72        | 16     | 1     |
| 1:A:344:VAL:CG1  | 1:A:346:LEU:HD21 | 0.42     | 2.45        | 3      | 2     |
| 1:A:373:PHE:CE1  | 1:A:375:ASN:HA   | 0.42     | 2.50        | 4      | 1     |
| 1:A:338:ILE:O    | 1:A:340:ALA:N    | 0.42     | 2.53        | 8      | 4     |
| 1:A:396:VAL:O    | 1:A:398:ASN:N    | 0.42     | 2.53        | 13     | 3     |
| 1:A:367:SER:O    | 1:A:370:SER:N    | 0.42     | 2.51        | 14     | 1     |
| 1:A:424:GLY:HA3  | 1:A:458:ILE:HD12 | 0.42     | 1.91        | 9      | 1     |
| 1:A:307:TRP:CD2  | 1:A:318:VAL:HB   | 0.42     | 2.50        | 17     | 1     |
| 1:A:437:ASN:O    | 1:A:438:LYS:C    | 0.42     | 2.58        | 17     | 1     |
| 1:A:337:GLU:HB3  | 1:A:344:VAL:HG12 | 0.42     | 1.92        | 20     | 1     |
| 1:A:354:LEU:O    | 1:A:360:PRO:CB   | 0.42     | 2.67        | 6      | 1     |
| 1:A:373:PHE:CE2  | 1:A:380:ILE:HG12 | 0.42     | 2.50        | 6      | 1     |
| 1:A:354:LEU:HD13 | 1:A:355:ILE:N    | 0.42     | 2.30        | 3      | 1     |
| 1:A:281:LEU:O    | 1:A:468:PHE:CE2  | 0.42     | 2.72        | 5      | 1     |
| 1:A:329:PRO:CB   | 1:A:348:LYS:HD3  | 0.42     | 2.44        | 16     | 1     |
| 1:A:343:GLN:CG   | 1:A:355:ILE:O    | 0.42     | 2.67        | 1      | 1     |
| 1:A:307:TRP:CE2  | 1:A:316:THR:OG1  | 0.42     | 2.72        | 14     | 1     |
| 1:A:389:PHE:O    | 1:A:391:ARG:CG   | 0.42     | 2.67        | 11     | 1     |
| 1:A:455:LEU:O    | 1:A:456:GLN:NE2  | 0.42     | 2.53        | 11     | 1     |
| 1:A:442:PHE:CZ   | 1:A:449:PHE:HB3  | 0.42     | 2.49        | 20     | 1     |
| 1:A:354:LEU:HD12 | 1:A:354:LEU:O    | 0.42     | 2.12        | 18     | 1     |
| 1:A:425:ILE:CG2  | 1:A:442:PHE:CD1  | 0.42     | 3.03        | 18     | 1     |
| 1:A:443:PHE:CZ   | 1:A:464:SER:HB2  | 0.42     | 2.49        | 18     | 1     |
| 1:A:396:VAL:O    | 1:A:397:ASP:CB   | 0.42     | 2.68        | 1      | 1     |
| 1:A:467:TRP:C    | 1:A:469:GLY:N    | 0.42     | 2.73        | 11     | 1     |
| 1:A:296:ASN:CG   | 1:A:296:ASN:O    | 0.42     | 2.58        | 3      | 1     |
| 1:A:369:HIS:CD2  | 1:A:369:HIS:C    | 0.42     | 2.92        | 3      | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:443:PHE:CE1  | 1:A:448:GLN:HB3  | 0.42     | 2.50        | 3      | 1     |
| 1:A:400:TYR:CD1  | 1:A:401:TRP:N    | 0.42     | 2.87        | 5      | 1     |
| 1:A:443:PHE:CD1  | 1:A:444:GLN:N    | 0.42     | 2.87        | 5      | 1     |
| 1:A:322:SER:C    | 1:A:324:LEU:N    | 0.42     | 2.70        | 19     | 1     |
| 1:A:354:LEU:HD23 | 1:A:361:GLU:HG2  | 0.42     | 1.90        | 16     | 1     |
| 1:A:368:ILE:O    | 1:A:370:SER:N    | 0.42     | 2.53        | 1      | 1     |
| 1:A:362:PRO:O    | 1:A:363:ASN:HB2  | 0.42     | 2.14        | 5      | 2     |
| 1:A:348:LYS:N    | 1:A:351:LYS:O    | 0.42     | 2.49        | 13     | 1     |
| 1:A:376:PHE:O    | 1:A:377:VAL:O    | 0.42     | 2.38        | 14     | 1     |
| 1:A:301:PHE:CZ   | 1:A:306:PHE:CE1  | 0.42     | 3.08        | 9      | 1     |
| 1:A:448:GLN:HG3  | 1:A:462:LEU:HD23 | 0.42     | 1.91        | 12     | 1     |
| 1:A:436:LYS:HD3  | 1:A:439:TYR:CD1  | 0.42     | 2.50        | 5      | 1     |
| 1:A:332:ILE:HG12 | 1:A:346:LEU:HD12 | 0.42     | 1.90        | 2      | 1     |
| 1:A:380:ILE:HG22 | 1:A:381:ASP:H    | 0.42     | 1.75        | 15     | 1     |
| 1:A:400:TYR:CG   | 1:A:400:TYR:O    | 0.42     | 2.73        | 9      | 3     |
| 1:A:469:GLY:O    | 1:A:470:CYS:SG   | 0.42     | 2.78        | 8      | 1     |
| 1:A:307:TRP:CD1  | 1:A:318:VAL:HG22 | 0.42     | 2.50        | 12     | 1     |
| 1:A:286:LEU:HD22 | 1:A:288:PHE:CZ   | 0.42     | 2.50        | 10     | 1     |
| 1:A:455:LEU:HD11 | 1:A:457:ARG:HB2  | 0.42     | 1.91        | 5      | 1     |
| 1:A:385:PHE:CG   | 1:A:386:ASN:N    | 0.41     | 2.87        | 2      | 1     |
| 1:A:300:PHE:CD1  | 1:A:301:PHE:N    | 0.41     | 2.88        | 18     | 1     |
| 1:A:422:PHE:CE1  | 1:A:451:TYR:CE2  | 0.41     | 3.08        | 18     | 1     |
| 1:A:433:PHE:CE1  | 1:A:441:TYR:HB3  | 0.41     | 2.50        | 18     | 1     |
| 1:A:444:GLN:CD   | 1:A:444:GLN:O    | 0.41     | 2.59        | 15     | 1     |
| 1:A:468:PHE:CE1  | 1:A:470:CYS:HB2  | 0.41     | 2.50        | 20     | 2     |
| 1:A:285:ASN:O    | 1:A:285:ASN:CG   | 0.41     | 2.58        | 14     | 1     |
| 1:A:431:ALA:C    | 1:A:432:VAL:HG13 | 0.41     | 2.35        | 14     | 1     |
| 1:A:352:TYR:O    | 1:A:352:TYR:CD1  | 0.41     | 2.73        | 3      | 2     |
| 1:A:369:HIS:HB2  | 1:A:373:PHE:CG   | 0.41     | 2.50        | 12     | 1     |
| 1:A:381:ASP:O    | 1:A:430:ASP:O    | 0.41     | 2.38        | 17     | 1     |
| 1:A:422:PHE:CB   | 1:A:425:ILE:HD11 | 0.41     | 2.45        | 11     | 1     |
| 1:A:399:GLN:O    | 1:A:418:ILE:CD1  | 0.41     | 2.68        | 10     | 1     |
| 1:A:357:ASN:O    | 1:A:358:LEU:CG   | 0.41     | 2.68        | 16     | 1     |
| 1:A:374:PRO:O    | 1:A:375:ASN:CG   | 0.41     | 2.58        | 16     | 1     |
| 1:A:281:LEU:HB3  | 1:A:468:PHE:CE2  | 0.41     | 2.50        | 16     | 1     |
| 1:A:343:GLN:OE1  | 1:A:345:PHE:CE1  | 0.41     | 2.72        | 8      | 1     |
| 1:A:356:SER:N    | 1:A:359:ARG:O    | 0.41     | 2.52        | 10     | 1     |
| 1:A:424:GLY:H    | 1:A:425:ILE:HD13 | 0.41     | 1.75        | 10     | 2     |
| 1:A:377:VAL:O    | 1:A:378:LYS:CB   | 0.41     | 2.68        | 3      | 1     |
| 1:A:296:ASN:N    | 1:A:296:ASN:OD1  | 0.41     | 2.53        | 16     | 1     |
| 1:A:321:ILE:C    | 1:A:323:SER:N    | 0.41     | 2.74        | 2      | 2     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:436:LYS:HG3  | 1:A:441:TYR:CE1  | 0.41     | 2.50        | 2      | 1     |
| 1:A:322:SER:O    | 1:A:325:TRP:O    | 0.41     | 2.38        | 15     | 1     |
| 1:A:296:ASN:OD1  | 1:A:296:ASN:C    | 0.41     | 2.56        | 14     | 1     |
| 1:A:425:ILE:HG12 | 1:A:442:PHE:CD2  | 0.41     | 2.50        | 9      | 1     |
| 1:A:391:ARG:HG2  | 1:A:392:THR:N    | 0.41     | 2.30        | 20     | 1     |
| 1:A:373:PHE:C    | 1:A:373:PHE:CD1  | 0.41     | 2.92        | 3      | 1     |
| 1:A:393:TYR:CE1  | 1:A:402:ARG:NE   | 0.41     | 2.88        | 16     | 1     |
| 1:A:307:TRP:CE3  | 1:A:307:TRP:HA   | 0.41     | 2.51        | 15     | 1     |
| 1:A:354:LEU:N    | 1:A:354:LEU:HD13 | 0.41     | 2.31        | 15     | 1     |
| 1:A:351:LYS:CB   | 1:A:366:LYS:O    | 0.41     | 2.69        | 13     | 1     |
| 1:A:462:LEU:CB   | 1:A:466:SER:HB3  | 0.41     | 2.45        | 7      | 1     |
| 1:A:358:LEU:HD12 | 1:A:358:LEU:O    | 0.41     | 2.16        | 12     | 1     |
| 1:A:349:ASP:O    | 1:A:378:LYS:O    | 0.41     | 2.39        | 10     | 1     |
| 1:A:368:ILE:C    | 1:A:370:SER:N    | 0.41     | 2.73        | 18     | 2     |
| 1:A:381:ASP:CG   | 1:A:429:ILE:O    | 0.41     | 2.59        | 4      | 3     |
| 1:A:362:PRO:C    | 1:A:363:ASN:CG   | 0.41     | 2.79        | 8      | 2     |
| 1:A:352:TYR:CE2  | 1:A:366:LYS:HB3  | 0.41     | 2.50        | 11     | 1     |
| 1:A:372:GLY:O    | 1:A:373:PHE:CD1  | 0.41     | 2.73        | 20     | 1     |
| 1:A:432:VAL:CG2  | 1:A:442:PHE:CD2  | 0.41     | 3.04        | 5      | 1     |
| 1:A:433:PHE:O    | 1:A:433:PHE:CG   | 0.41     | 2.73        | 18     | 1     |
| 1:A:432:VAL:HG23 | 1:A:442:PHE:CE1  | 0.41     | 2.48        | 1      | 1     |
| 1:A:442:PHE:HB2  | 1:A:451:TYR:CE1  | 0.41     | 2.50        | 13     | 1     |
| 1:A:330:SER:O    | 1:A:332:ILE:N    | 0.41     | 2.54        | 20     | 1     |
| 1:A:364:TYR:CZ   | 1:A:366:LYS:HE3  | 0.41     | 2.49        | 3      | 1     |
| 1:A:389:PHE:CD2  | 1:A:402:ARG:NH1  | 0.41     | 2.88        | 19     | 1     |
| 1:A:354:LEU:CD2  | 1:A:361:GLU:CG   | 0.41     | 2.99        | 16     | 1     |
| 1:A:445:GLY:O    | 1:A:447:ASN:CG   | 0.41     | 2.59        | 16     | 1     |
| 1:A:430:ASP:OD1  | 1:A:430:ASP:N    | 0.41     | 2.54        | 7      | 1     |
| 1:A:321:ILE:HD12 | 1:A:330:SER:HB3  | 0.41     | 1.93        | 10     | 1     |
| 1:A:305:PHE:CD2  | 1:A:318:VAL:HB   | 0.41     | 2.50        | 19     | 1     |
| 1:A:321:ILE:O    | 1:A:323:SER:N    | 0.41     | 2.53        | 2      | 1     |
| 1:A:305:PHE:CB   | 1:A:307:TRP:CH2  | 0.41     | 3.04        | 18     | 1     |
| 1:A:436:LYS:HD3  | 1:A:441:TYR:CD1  | 0.41     | 2.50        | 7      | 1     |
| 1:A:398:ASN:O    | 1:A:398:ASN:OD1  | 0.41     | 2.38        | 17     | 1     |
| 1:A:332:ILE:CG2  | 1:A:346:LEU:HD12 | 0.41     | 2.45        | 11     | 1     |
| 1:A:419:THR:O    | 1:A:423:GLN:CG   | 0.41     | 2.69        | 11     | 1     |
| 1:A:287:SER:O    | 1:A:302:LYS:CE   | 0.41     | 2.68        | 6      | 1     |
| 1:A:352:TYR:CE2  | 1:A:368:ILE:HG22 | 0.41     | 2.51        | 6      | 1     |
| 1:A:368:ILE:O    | 1:A:373:PHE:N    | 0.41     | 2.54        | 6      | 1     |
| 1:A:396:VAL:CG1  | 1:A:401:TRP:CZ3  | 0.41     | 3.03        | 5      | 1     |
| 1:A:398:ASN:CG   | 1:A:398:ASN:O    | 0.41     | 2.59        | 19     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:374:PRO:HD2  | 1:A:377:VAL:CG1  | 0.41     | 2.45        | 16     | 1     |
| 1:A:286:LEU:CD2  | 1:A:307:TRP:CH2  | 0.41     | 3.04        | 2      | 1     |
| 1:A:302:LYS:O    | 1:A:305:PHE:N    | 0.41     | 2.54        | 1      | 1     |
| 1:A:467:TRP:HA   | 1:A:467:TRP:CE3  | 0.41     | 2.50        | 4      | 1     |
| 1:A:282:CYS:CA   | 1:A:470:CYS:SG   | 0.41     | 3.08        | 13     | 1     |
| 1:A:349:ASP:O    | 1:A:350:ASP:CB   | 0.41     | 2.68        | 13     | 1     |
| 1:A:424:GLY:HA3  | 1:A:458:ILE:CD1  | 0.41     | 2.46        | 8      | 1     |
| 1:A:436:LYS:HE2  | 1:A:441:TYR:CE1  | 0.41     | 2.51        | 9      | 1     |
| 1:A:306:PHE:O    | 1:A:319:ASN:O    | 0.41     | 2.38        | 9      | 1     |
| 1:A:328:LEU:CD1  | 1:A:329:PRO:HD2  | 0.41     | 2.46        | 11     | 1     |
| 1:A:306:PHE:CE1  | 1:A:319:ASN:HB2  | 0.41     | 2.51        | 10     | 1     |
| 1:A:329:PRO:HG3  | 1:A:353:TRP:CH2  | 0.41     | 2.51        | 10     | 1     |
| 1:A:464:SER:O    | 1:A:465:ASN:CG   | 0.41     | 2.59        | 10     | 1     |
| 1:A:453:PHE:O    | 1:A:454:LEU:C    | 0.41     | 2.59        | 19     | 2     |
| 1:A:350:ASP:OD2  | 1:A:350:ASP:O    | 0.41     | 2.39        | 20     | 1     |
| 1:A:399:GLN:CG   | 1:A:416:LYS:O    | 0.41     | 2.69        | 20     | 1     |
| 1:A:281:LEU:HB3  | 1:A:468:PHE:CD2  | 0.41     | 2.50        | 5      | 1     |
| 1:A:393:TYR:CE1  | 1:A:402:ARG:NH1  | 0.41     | 2.89        | 19     | 1     |
| 1:A:395:PHE:CE1  | 1:A:432:VAL:HG11 | 0.41     | 2.50        | 2      | 1     |
| 1:A:290:ALA:O    | 1:A:291:VAL:HG13 | 0.41     | 2.15        | 10     | 1     |
| 1:A:304:ARG:O    | 1:A:320:LEU:CD1  | 0.41     | 2.66        | 20     | 1     |
| 1:A:324:LEU:O    | 1:A:325:TRP:C    | 0.40     | 2.60        | 16     | 1     |
| 1:A:455:LEU:C    | 1:A:456:GLN:OE1  | 0.40     | 2.60        | 2      | 1     |
| 1:A:464:SER:C    | 1:A:466:SER:N    | 0.40     | 2.74        | 18     | 1     |
| 1:A:420:LYS:O    | 1:A:421:ASN:C    | 0.40     | 2.59        | 15     | 1     |
| 1:A:450:GLU:OE1  | 1:A:451:TYR:O    | 0.40     | 2.40        | 14     | 1     |
| 1:A:308:LEU:HD23 | 1:A:317:SER:CB   | 0.40     | 2.46        | 16     | 1     |
| 1:A:376:PHE:O    | 1:A:377:VAL:C    | 0.40     | 2.59        | 16     | 1     |
| 1:A:462:LEU:HG   | 1:A:463:LYS:N    | 0.40     | 2.32        | 15     | 1     |
| 1:A:344:VAL:HG12 | 1:A:346:LEU:HD23 | 0.40     | 1.93        | 14     | 1     |
| 1:A:368:ILE:HD11 | 1:A:377:VAL:HG21 | 0.40     | 1.93        | 9      | 1     |
| 1:A:334:ALA:HB3  | 1:A:347:PHE:HB2  | 0.40     | 1.91        | 11     | 1     |
| 1:A:402:ARG:HB3  | 1:A:402:ARG:CZ   | 0.40     | 2.46        | 11     | 1     |
| 1:A:286:LEU:CD2  | 1:A:288:PHE:CE2  | 0.40     | 3.05        | 10     | 1     |
| 1:A:465:ASN:O    | 1:A:470:CYS:C    | 0.40     | 2.59        | 10     | 2     |
| 1:A:299:PHE:CZ   | 1:A:308:LEU:HD11 | 0.40     | 2.51        | 20     | 1     |
| 1:A:400:TYR:CZ   | 1:A:416:LYS:HB2  | 0.40     | 2.51        | 20     | 1     |
| 1:A:455:LEU:O    | 1:A:456:GLN:CD   | 0.40     | 2.59        | 6      | 1     |
| 1:A:452:ASP:OD1  | 1:A:454:LEU:CB   | 0.40     | 2.69        | 18     | 1     |
| 1:A:432:VAL:HA   | 1:A:442:PHE:CG   | 0.40     | 2.51        | 15     | 1     |
| 1:A:383:ALA:CB   | 1:A:394:PHE:CE1  | 0.40     | 3.05        | 13     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:419:THR:O    | 1:A:422:PHE:C    | 0.40     | 2.60        | 13     | 1     |
| 1:A:345:PHE:CE1  | 1:A:354:LEU:HD13 | 0.40     | 2.50        | 20     | 1     |
| 1:A:433:PHE:CG   | 1:A:434:TYR:N    | 0.40     | 2.89        | 6      | 1     |
| 1:A:303:ASP:O    | 1:A:304:ARG:HB2  | 0.40     | 2.17        | 16     | 2     |
| 1:A:429:ILE:HD11 | 1:A:442:PHE:CG   | 0.40     | 2.51        | 16     | 1     |
| 1:A:455:LEU:C    | 1:A:456:GLN:CD   | 0.40     | 2.80        | 16     | 1     |
| 1:A:462:LEU:HD12 | 1:A:466:SER:HB2  | 0.40     | 1.92        | 16     | 1     |
| 1:A:298:ILE:O    | 1:A:308:LEU:HD12 | 0.40     | 2.15        | 18     | 1     |
| 1:A:291:VAL:O    | 1:A:335:ALA:O    | 0.40     | 2.40        | 15     | 1     |
| 1:A:445:GLY:O    | 1:A:446:SER:CB   | 0.40     | 2.68        | 15     | 1     |
| 1:A:290:ALA:HA   | 1:A:431:ALA:HB2  | 0.40     | 1.93        | 17     | 1     |
| 1:A:439:TYR:CD2  | 1:A:452:ASP:OD1  | 0.40     | 2.74        | 20     | 1     |
| 1:A:300:PHE:CE1  | 1:A:301:PHE:O    | 0.40     | 2.75        | 18     | 1     |
| 1:A:369:HIS:C    | 1:A:371:PHE:N    | 0.40     | 2.74        | 1      | 1     |
| 1:A:432:VAL:HG23 | 1:A:440:TYR:CE1  | 0.40     | 2.51        | 15     | 1     |
| 1:A:294:VAL:HG23 | 1:A:297:LYS:CB   | 0.40     | 2.45        | 14     | 1     |
| 1:A:364:TYR:CD2  | 1:A:366:LYS:HG2  | 0.40     | 2.51        | 14     | 1     |
| 1:A:298:ILE:HD12 | 1:A:300:PHE:CE2  | 0.40     | 2.52        | 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     | 189/194 (97%)   | 138±5 (73±3%) | 38±5 (20±3%) | 13±3 (7±1%) | 3           | 18 |
| All | All   | 3780/3880 (97%) | 2753 (73%)    | 767 (20%)    | 260 (7%)    | 3           | 18 |

All 48 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     | 326 | PRO  | 20             |
| 1   | A     | 378 | LYS  | 16             |
| 1   | A     | 413 | GLY  | 15             |
| 1   | A     | 455 | LEU  | 14             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 303 | ASP  | 13             |
| 1   | A     | 372 | GLY  | 12             |
| 1   | A     | 311 | SER  | 12             |
| 1   | A     | 436 | LYS  | 11             |
| 1   | A     | 373 | PHE  | 10             |
| 1   | A     | 282 | CYS  | 10             |
| 1   | A     | 285 | ASN  | 9              |
| 1   | A     | 376 | PHE  | 9              |
| 1   | A     | 310 | VAL  | 9              |
| 1   | A     | 374 | PRO  | 8              |
| 1   | A     | 371 | PHE  | 8              |
| 1   | A     | 425 | ILE  | 7              |
| 1   | A     | 438 | LYS  | 6              |
| 1   | A     | 363 | ASN  | 6              |
| 1   | A     | 467 | TRP  | 6              |
| 1   | A     | 377 | VAL  | 5              |
| 1   | A     | 295 | GLY  | 4              |
| 1   | A     | 332 | ILE  | 4              |
| 1   | A     | 321 | ILE  | 3              |
| 1   | A     | 419 | THR  | 3              |
| 1   | A     | 412 | PRO  | 3              |
| 1   | A     | 446 | SER  | 3              |
| 1   | A     | 375 | ASN  | 3              |
| 1   | A     | 358 | LEU  | 3              |
| 1   | A     | 468 | PHE  | 2              |
| 1   | A     | 331 | GLY  | 2              |
| 1   | A     | 389 | PHE  | 2              |
| 1   | A     | 342 | ASN  | 2              |
| 1   | A     | 465 | ASN  | 2              |
| 1   | A     | 418 | ILE  | 2              |
| 1   | A     | 408 | GLN  | 2              |
| 1   | A     | 397 | ASP  | 2              |
| 1   | A     | 302 | LYS  | 1              |
| 1   | A     | 330 | SER  | 1              |
| 1   | A     | 312 | GLU  | 1              |
| 1   | A     | 350 | ASP  | 1              |
| 1   | A     | 294 | VAL  | 1              |
| 1   | A     | 314 | PRO  | 1              |
| 1   | A     | 430 | ASP  | 1              |
| 1   | A     | 349 | ASP  | 1              |
| 1   | A     | 432 | VAL  | 1              |
| 1   | A     | 456 | GLN  | 1              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 340 | ALA  | 1              |
| 1   | A     | 359 | ARG  | 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     | 175/178 (98%)   | 128±5 (73±3%) | 47±5 (27±3%) | 2           | 22 |
| All | All   | 3500/3560 (98%) | 2556 (73%)    | 944 (27%)    | 2           | 22 |

All 139 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     | 304 | ARG  | 18             |
| 1   | A     | 410 | MET  | 18             |
| 1   | A     | 364 | TYR  | 17             |
| 1   | A     | 407 | ARG  | 16             |
| 1   | A     | 378 | LYS  | 16             |
| 1   | A     | 438 | LYS  | 16             |
| 1   | A     | 285 | ASN  | 16             |
| 1   | A     | 358 | LEU  | 15             |
| 1   | A     | 404 | ASP  | 15             |
| 1   | A     | 348 | LYS  | 15             |
| 1   | A     | 325 | TRP  | 15             |
| 1   | A     | 366 | LYS  | 14             |
| 1   | A     | 428 | LYS  | 14             |
| 1   | A     | 417 | LEU  | 14             |
| 1   | A     | 320 | LEU  | 14             |
| 1   | A     | 460 | LYS  | 14             |
| 1   | A     | 371 | PHE  | 14             |
| 1   | A     | 463 | LYS  | 13             |
| 1   | A     | 317 | SER  | 13             |
| 1   | A     | 359 | ARG  | 13             |
| 1   | A     | 381 | ASP  | 13             |
| 1   | A     | 470 | CYS  | 13             |
| 1   | A     | 302 | LYS  | 13             |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 354 | LEU  | 12             |
| 1   | A     | 397 | ASP  | 12             |
| 1   | A     | 411 | ASP  | 12             |
| 1   | A     | 457 | ARG  | 11             |
| 1   | A     | 376 | PHE  | 11             |
| 1   | A     | 289 | ASP  | 11             |
| 1   | A     | 308 | LEU  | 11             |
| 1   | A     | 443 | PHE  | 11             |
| 1   | A     | 430 | ASP  | 11             |
| 1   | A     | 369 | HIS  | 11             |
| 1   | A     | 313 | ARG  | 11             |
| 1   | A     | 379 | LYS  | 10             |
| 1   | A     | 447 | ASN  | 10             |
| 1   | A     | 323 | SER  | 10             |
| 1   | A     | 283 | ASP  | 10             |
| 1   | A     | 408 | GLN  | 10             |
| 1   | A     | 337 | GLU  | 10             |
| 1   | A     | 388 | ARG  | 9              |
| 1   | A     | 448 | GLN  | 9              |
| 1   | A     | 286 | LEU  | 9              |
| 1   | A     | 389 | PHE  | 9              |
| 1   | A     | 339 | GLU  | 9              |
| 1   | A     | 315 | LYS  | 9              |
| 1   | A     | 425 | ILE  | 9              |
| 1   | A     | 455 | LEU  | 9              |
| 1   | A     | 282 | CYS  | 9              |
| 1   | A     | 436 | LYS  | 9              |
| 1   | A     | 370 | SER  | 9              |
| 1   | A     | 444 | GLN  | 8              |
| 1   | A     | 324 | LEU  | 8              |
| 1   | A     | 406 | ARG  | 8              |
| 1   | A     | 386 | ASN  | 8              |
| 1   | A     | 467 | TRP  | 8              |
| 1   | A     | 367 | SER  | 7              |
| 1   | A     | 409 | MET  | 7              |
| 1   | A     | 450 | GLU  | 7              |
| 1   | A     | 399 | GLN  | 7              |
| 1   | A     | 400 | TYR  | 7              |
| 1   | A     | 303 | ASP  | 7              |
| 1   | A     | 435 | SER  | 7              |
| 1   | A     | 401 | TRP  | 7              |
| 1   | A     | 281 | LEU  | 7              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 309 | LYS  | 7              |
| 1   | A     | 405 | GLU  | 7              |
| 1   | A     | 466 | SER  | 6              |
| 1   | A     | 464 | SER  | 6              |
| 1   | A     | 357 | ASN  | 6              |
| 1   | A     | 341 | ARG  | 6              |
| 1   | A     | 333 | GLU  | 6              |
| 1   | A     | 310 | VAL  | 6              |
| 1   | A     | 328 | LEU  | 5              |
| 1   | A     | 462 | LEU  | 5              |
| 1   | A     | 345 | PHE  | 5              |
| 1   | A     | 429 | ILE  | 5              |
| 1   | A     | 322 | SER  | 5              |
| 1   | A     | 312 | GLU  | 5              |
| 1   | A     | 330 | SER  | 5              |
| 1   | A     | 361 | GLU  | 4              |
| 1   | A     | 336 | TYR  | 4              |
| 1   | A     | 423 | GLN  | 4              |
| 1   | A     | 377 | VAL  | 4              |
| 1   | A     | 343 | GLN  | 4              |
| 1   | A     | 297 | LYS  | 4              |
| 1   | A     | 419 | THR  | 4              |
| 1   | A     | 352 | TYR  | 4              |
| 1   | A     | 363 | ASN  | 4              |
| 1   | A     | 394 | PHE  | 4              |
| 1   | A     | 452 | ASP  | 4              |
| 1   | A     | 338 | ILE  | 4              |
| 1   | A     | 319 | ASN  | 4              |
| 1   | A     | 327 | THR  | 4              |
| 1   | A     | 311 | SER  | 4              |
| 1   | A     | 451 | TYR  | 3              |
| 1   | A     | 446 | SER  | 3              |
| 1   | A     | 292 | THR  | 3              |
| 1   | A     | 307 | TRP  | 3              |
| 1   | A     | 349 | ASP  | 3              |
| 1   | A     | 356 | SER  | 3              |
| 1   | A     | 300 | PHE  | 3              |
| 1   | A     | 402 | ARG  | 3              |
| 1   | A     | 441 | TYR  | 2              |
| 1   | A     | 468 | PHE  | 2              |
| 1   | A     | 346 | LEU  | 2              |
| 1   | A     | 368 | ILE  | 2              |

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| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 418 | ILE  | 2              |
| 1   | A     | 375 | ASN  | 2              |
| 1   | A     | 353 | TRP  | 2              |
| 1   | A     | 296 | ASN  | 2              |
| 1   | A     | 391 | ARG  | 2              |
| 1   | A     | 414 | TYR  | 2              |
| 1   | A     | 421 | ASN  | 2              |
| 1   | A     | 306 | PHE  | 2              |
| 1   | A     | 342 | ASN  | 2              |
| 1   | A     | 440 | TYR  | 2              |
| 1   | A     | 293 | THR  | 1              |
| 1   | A     | 305 | PHE  | 1              |
| 1   | A     | 459 | THR  | 1              |
| 1   | A     | 456 | GLN  | 1              |
| 1   | A     | 385 | PHE  | 1              |
| 1   | A     | 321 | ILE  | 1              |
| 1   | A     | 298 | ILE  | 1              |
| 1   | A     | 396 | VAL  | 1              |
| 1   | A     | 355 | ILE  | 1              |
| 1   | A     | 434 | TYR  | 1              |
| 1   | A     | 373 | PHE  | 1              |
| 1   | A     | 301 | PHE  | 1              |
| 1   | A     | 318 | VAL  | 1              |
| 1   | A     | 442 | PHE  | 1              |
| 1   | A     | 384 | VAL  | 1              |
| 1   | A     | 432 | VAL  | 1              |
| 1   | A     | 347 | PHE  | 1              |
| 1   | A     | 433 | PHE  | 1              |
| 1   | A     | 437 | ASN  | 1              |
| 1   | A     | 287 | SER  | 1              |
| 1   | A     | 350 | ASP  | 1              |
| 1   | A     | 393 | TYR  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 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 79% for the well-defined parts and 78% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 7414

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                  | 2173 |
| Number of shifts mapped to atoms        | 2173 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 31   |

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 192      | $2.92 \pm 0.14$                 | Should be applied          |
| $^{13}\text{C}_\beta$  | 184      | $3.19 \pm 0.17$                 | Should be applied          |
| $^{13}\text{C}'$       | 176      | $3.15 \pm 0.12$                 | Should be applied          |
| $^{15}\text{N}$        | 179      | $0.21 \pm 0.22$                 | None needed ( $< 0.5$ ppm) |

#### 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 77%, i.e. 1972 atoms were assigned a chemical shift out of a possible 2546. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$   | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|----------------|-----------------|-----------------|
| Backbone  | 909/926 (98%)  | 367/368 (100%) | 364/380 (96%)   | 178/178 (100%)  |
| Sidechain | 992/1250 (79%) | 596/746 (80%)  | 380/438 (87%)   | 16/66 (24%)     |

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|          | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|----------|-----------------|----------------------|-----------------------|-----------------------|
| Aromatic | 71/370 (19%)    | 66/196 (34%)         | 0/167 (0%)            | 5/7 (71%)             |
| Overall  | 1972/2546 (77%) | 1029/1310 (79%)      | 744/985 (76%)         | 199/251 (79%)         |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1991 atoms were assigned a chemical shift out of a possible 2590. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | <b>Total</b>    | <b><sup>1</sup>H</b> | <b><sup>13</sup>C</b> | <b><sup>15</sup>N</b> |
|-----------|-----------------|----------------------|-----------------------|-----------------------|
| Backbone  | 917/944 (97%)   | 370/375 (99%)        | 368/388 (95%)         | 179/181 (99%)         |
| Sidechain | 1003/1276 (79%) | 603/762 (79%)        | 384/448 (86%)         | 16/66 (24%)           |
| Aromatic  | 71/370 (19%)    | 66/196 (34%)         | 0/167 (0%)            | 5/7 (71%)             |
| Overall   | 1991/2590 (77%) | 1039/1333 (78%)      | 752/1003 (75%)        | 200/254 (79%)         |

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1   | A     | 359 | ARG  | CD   | 23.47      | 47.57 – 38.77       | -22.4   |
| 1   | A     | 359 | ARG  | CG   | 40.33      | 33.23 – 21.23       | 10.9    |
| 1   | A     | 392 | THR  | HG23 | -1.21      | 2.29 – -0.01        | -10.2   |
| 1   | A     | 392 | THR  | HG21 | -1.21      | 2.29 – -0.01        | -10.2   |
| 1   | A     | 392 | THR  | HG22 | -1.21      | 2.29 – -0.01        | -10.2   |
| 1   | A     | 369 | HIS  | HD2  | 10.35      | 9.28 – 4.78         | 7.4     |
| 1   | A     | 450 | GLU  | HG3  | 0.75       | 3.31 – 1.21         | -7.2    |
| 1   | A     | 415 | PRO  | HB3  | -0.47      | 3.81 – 0.21         | -6.9    |
| 1   | A     | 410 | MET  | CG   | 23.73      | 38.33 – 25.73       | -6.6    |
| 1   | A     | 365 | PRO  | CG   | 20.18      | 32.66 – 21.76       | -6.4    |
| 1   | A     | 365 | PRO  | HB3  | -0.30      | 3.81 – 0.21         | -6.4    |
| 1   | A     | 359 | ARG  | HD2  | 1.65       | 4.27 – 1.97         | -6.4    |
| 1   | A     | 298 | ILE  | HG21 | -0.94      | 2.13 – -0.57        | -6.4    |
| 1   | A     | 298 | ILE  | HG23 | -0.94      | 2.13 – -0.57        | -6.4    |
| 1   | A     | 298 | ILE  | HG22 | -0.94      | 2.13 – -0.57        | -6.4    |
| 1   | A     | 416 | LYS  | HE3  | 1.70       | 3.86 – 1.96         | -6.3    |
| 1   | A     | 297 | LYS  | CD   | 21.56      | 34.86 – 23.06       | -6.3    |
| 1   | A     | 359 | ARG  | HD3  | 1.54       | 4.36 – 1.86         | -6.3    |
| 1   | A     | 359 | ARG  | HG2  | 3.19       | 2.92 – 0.22         | 6.0     |
| 1   | A     | 402 | ARG  | CG   | 20.12      | 33.23 – 21.23       | -5.9    |
| 1   | A     | 425 | ILE  | HG23 | -0.78      | 2.13 – -0.57        | -5.8    |
| 1   | A     | 425 | ILE  | HG22 | -0.78      | 2.13 – -0.57        | -5.8    |

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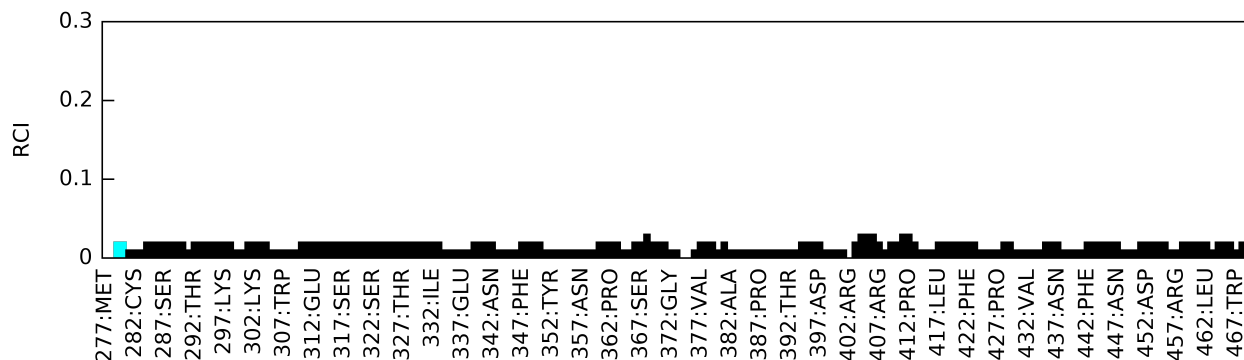
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| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1   | A     | 425 | ILE  | HG21 | -0.78      | 2.13 – -0.57        | -5.8    |
| 1   | A     | 319 | ASN  | HB3  | 0.88       | 4.41 – 1.11         | -5.7    |
| 1   | A     | 415 | PRO  | CG   | 21.23      | 32.66 – 21.76       | -5.5    |
| 1   | A     | 359 | ARG  | HG3  | 3.13       | 3.00 – 0.10         | 5.5     |
| 1   | A     | 427 | PRO  | CG   | 21.31      | 32.66 – 21.76       | -5.4    |
| 1   | A     | 448 | GLN  | HG3  | 0.82       | 3.75 – 0.85         | -5.1    |
| 1   | A     | 380 | ILE  | HD13 | -0.79      | 2.13 – -0.77        | -5.1    |
| 1   | A     | 380 | ILE  | HD12 | -0.79      | 2.13 – -0.77        | -5.1    |
| 1   | A     | 380 | ILE  | HD11 | -0.79      | 2.13 – -0.77        | -5.1    |

### 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.

Random coil index (RCI) for chain A:



## 7.2 Chemical shift list 2

File name: BMRB entry 15578

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

### 7.2.1 Bookkeeping [i](#)

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

|                        |      |
|------------------------|------|
| Total number of shifts | 3693 |
|------------------------|------|



|   |      |
|---|------|
| Number of shifts mapped to atoms        | 2080 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 1613 |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 19   |

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 1613 occurrences are reported below.

| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 152 | ARG  | CD   | 40.569     | 0.3         | 1         |
| A     | 126 | SER  | HB3  | 3.839      | 0.02        | 2         |
| A     | 68  | HIS  | HB2  | 2.02       | 0.02        | 2         |
| A     | 126 | SER  | C    | 170.638    | 0.3         | 1         |
| A     | 109 | PHE  | H    | 9.128      | 0.02        | 1         |
| A     | 76  | ILE  | HD12 | 0.903      | 0.02        | 1         |
| A     | 92  | HIS  | CB   | 31.092     | 0.3         | 1         |
| A     | 87  | ILE  | HG13 | 0.429      | 0.02        | 2         |
| A     | 84  | GLY  | H    | 5.621      | 0.02        | 1         |
| A     | 56  | LEU  | H    | 7.552      | 0.02        | 1         |
| A     | 36  | VAL  | HG22 | 0.401      | 0.02        | 1         |
| A     | 54  | ASP  | HA   | 4.421      | 0.02        | 1         |
| A     | 43  | LEU  | HB2  | 2.013      | 0.02        | 1         |
| A     | 37  | TRP  | NE1  | 128.128    | 0.3         | 1         |
| A     | 75  | GLY  | C    | 171.758    | 0.3         | 1         |
| A     | 78  | ALA  | HB1  | 1.003      | 0.02        | 1         |
| A     | 108 | LEU  | CA   | 55.908     | 0.3         | 1         |
| A     | 83  | PRO  | CD   | 47.677     | 0.3         | 1         |
| A     | 70  | PHE  | CA   | 54.14      | 0.3         | 1         |
| A     | 55  | ILE  | CG1  | 23.524     | 0.3         | 1         |
| A     | 73  | LYS  | C    | 175.036    | 0.3         | 1         |
| A     | 108 | LEU  | HD11 | 0.65       | 0.02        | 1         |
| A     | 55  | ILE  | HG13 | 1.233      | 0.02        | 2         |
| A     | 151 | ILE  | HG21 | 0.759      | 0.02        | 1         |
| A     | 113 | VAL  | HG22 | 0.012      | 0.02        | 1         |
| A     | 59  | PHE  | C    | 173.396    | 0.3         | 1         |
| A     | 42  | PRO  | CB   | 29.517     | 0.3         | 1         |
| A     | 21  | MET  | CA   | 50.542     | 0.3         | 1         |
| A     | 110 | LEU  | HD23 | 0.691      | 0.02        | 1         |
| A     | 110 | LEU  | CA   | 55.112     | 0.3         | 1         |
| A     | 124 | HIS  | CA   | 52.444     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 12  | TYR  | H    | 8.546      | 0.02        | 1         |
| A     | 156 | SER  | HA   | 4.169      | 0.02        | 1         |
| A     | 91  | ALA  | HB2  | 0.905      | 0.02        | 1         |
| A     | 38  | SER  | CA   | 58.68      | 0.3         | 1         |
| A     | 67  | ASP  | N    | 120.204    | 0.3         | 1         |
| A     | 10  | ILE  | HG23 | 0.276      | 0.02        | 1         |
| A     | 28  | TYR  | HA   | 4.088      | 0.02        | 1         |
| A     | 54  | ASP  | CB   | 38.363     | 0.3         | 1         |
| A     | 157 | LEU  | HD22 | 0.532      | 0.02        | 1         |
| A     | 30  | ILE  | CG1  | 24.43      | 0.3         | 1         |
| A     | 144 | PHE  | C    | 171.789    | 0.3         | 1         |
| A     | 125 | SER  | CA   | 52.441     | 0.3         | 1         |
| A     | 17  | TYR  | CB   | 36.071     | 0.3         | 1         |
| A     | 21  | MET  | HE2  | 0.306      | 0.02        | 1         |
| A     | 52  | MET  | N    | 119.106    | 0.3         | 1         |
| A     | 16  | ASN  | HB3  | 2.796      | 0.02        | 2         |
| A     | 30  | ILE  | N    | 113.835    | 0.3         | 1         |
| A     | 43  | LEU  | H    | 7.204      | 0.02        | 1         |
| A     | 106 | THR  | CG2  | 21.791     | 0.3         | 1         |
| A     | 81  | PHE  | CA   | 53.974     | 0.3         | 1         |
| A     | 146 | LEU  | C    | 174.323    | 0.3         | 1         |
| A     | 152 | ARG  | HG2  | 1.65       | 0.02        | 2         |
| A     | 87  | ILE  | C    | 171.613    | 0.3         | 1         |
| A     | 85  | SER  | CB   | 61.644     | 0.3         | 1         |
| A     | 18  | THR  | N    | 115.752    | 0.3         | 1         |
| A     | 9   | TYR  | C    | 171.18     | 0.3         | 1         |
| A     | 120 | LEU  | H    | 7.639      | 0.02        | 1         |
| A     | 127 | ASP  | C    | 171.04     | 0.3         | 1         |
| A     | 75  | GLY  | CA   | 43.631     | 0.3         | 1         |
| A     | 133 | PHE  | H    | 7.992      | 0.02        | 1         |
| A     | 134 | PRO  | CB   | 24.689     | 0.3         | 1         |
| A     | 120 | LEU  | HG   | 1.915      | 0.02        | 1         |
| A     | 30  | ILE  | HG12 | 1.547      | 0.02        | 2         |
| A     | 116 | ILE  | HD13 | -0.609     | 0.02        | 1         |
| A     | 103 | SER  | CA   | 52.091     | 0.3         | 1         |
| A     | 85  | SER  | HB2  | 4.006      | 0.02        | 2         |
| A     | 103 | SER  | HA   | 4.026      | 0.02        | 1         |
| A     | 59  | PHE  | CA   | 54.085     | 0.3         | 1         |
| A     | 6   | ARG  | H    | 7.458      | 0.02        | 1         |
| A     | 100 | THR  | CA   | 52.624     | 0.3         | 1         |
| A     | 57  | VAL  | CA   | 59.008     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 31  | ARG  | CB   | 27.322     | 0.3         | 1         |
| A     | 14  | ILE  | CD1  | 10.326     | 0.3         | 1         |
| A     | 73  | LYS  | HG3  | 1.194      | 0.02        | 2         |
| A     | 12  | TYR  | CB   | 40.428     | 0.3         | 1         |
| A     | 106 | THR  | HG23 | 0.203      | 0.02        | 1         |
| A     | 55  | ILE  | HD11 | 0.996      | 0.02        | 1         |
| A     | 70  | PHE  | N    | 120.039    | 0.3         | 1         |
| A     | 69  | ALA  | N    | 123.252    | 0.3         | 1         |
| A     | 111 | THR  | HG23 | 1.254      | 0.02        | 1         |
| A     | 39  | ASN  | HB3  | 2.802      | 0.02        | 2         |
| A     | 114 | HIS  | N    | 117.899    | 0.3         | 1         |
| A     | 89  | GLY  | H    | 7.783      | 0.02        | 1         |
| A     | 128 | PRO  | HG3  | 1.493      | 0.02        | 2         |
| A     | 112 | ALA  | CB   | 14.414     | 0.3         | 1         |
| A     | 32  | LYS  | CE   | 38.848     | 0.3         | 1         |
| A     | 87  | ILE  | CA   | 59.1       | 0.3         | 1         |
| A     | 13  | ARG  | HD2  | 2.89       | 0.02        | 1         |
| A     | 133 | PHE  | CA   | 53.846     | 0.3         | 1         |
| A     | 47  | LYS  | CD   | 27.337     | 0.3         | 1         |
| A     | 125 | SER  | HB2  | 4.26       | 0.02        | 2         |
| A     | 47  | LYS  | HA   | 3.314      | 0.02        | 1         |
| A     | 127 | ASP  | CA   | 48.143     | 0.3         | 1         |
| A     | 105 | GLY  | HA2  | 3.914      | 0.02        | 2         |
| A     | 25  | ASP  | HB3  | 2.515      | 0.02        | 2         |
| A     | 83  | PRO  | HG2  | 1.861      | 0.02        | 1         |
| A     | 40  | VAL  | CG1  | 18.555     | 0.3         | 1         |
| A     | 120 | LEU  | CB   | 39.402     | 0.3         | 1         |
| A     | 77  | LEU  | HD21 | 0.181      | 0.02        | 1         |
| A     | 152 | ARG  | CB   | 27.236     | 0.3         | 1         |
| A     | 21  | MET  | HB2  | 2.157      | 0.02        | 2         |
| A     | 18  | THR  | HB   | 3.739      | 0.02        | 1         |
| A     | 97  | GLU  | CA   | 53.325     | 0.3         | 1         |
| A     | 30  | ILE  | CA   | 59.172     | 0.3         | 1         |
| A     | 110 | LEU  | HD12 | 0.421      | 0.02        | 1         |
| A     | 69  | ALA  | C    | 177.582    | 0.3         | 1         |
| A     | 57  | VAL  | C    | 172.353    | 0.3         | 1         |
| A     | 135 | THR  | HA   | 4.538      | 0.02        | 1         |
| A     | 131 | VAL  | HG21 | 0.934      | 0.02        | 1         |
| A     | 4   | VAL  | HG12 | 0.416      | 0.02        | 1         |
| A     | 66  | ASP  | HA   | 4.946      | 0.02        | 1         |
| A     | 49  | ASN  | HD22 | 7.584      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 5   | TRP  | CB   | 25.732     | 0.3         | 1         |
| A     | 75  | GLY  | N    | 110.629    | 0.3         | 1         |
| A     | 23  | ARG  | HA   | 3.648      | 0.02        | 1         |
| A     | 154 | ILE  | HA   | 4.415      | 0.02        | 1         |
| A     | 23  | ARG  | CG   | 23.803     | 0.3         | 1         |
| A     | 151 | ILE  | CG1  | 28.01      | 0.3         | 1         |
| A     | 141 | ILE  | HG21 | 0.923      | 0.02        | 1         |
| A     | 37  | TRP  | HA   | 4.688      | 0.02        | 1         |
| A     | 35  | GLN  | HE22 | 6.887      | 0.02        | 1         |
| A     | 102 | HIS  | CB   | 28.205     | 0.3         | 1         |
| A     | 90  | ASP  | N    | 122.517    | 0.3         | 1         |
| A     | 53  | ALA  | CB   | 19.466     | 0.3         | 1         |
| A     | 152 | ARG  | HB2  | 1.85       | 0.02        | 2         |
| A     | 77  | LEU  | HG   | 1.599      | 0.02        | 1         |
| A     | 23  | ARG  | HG3  | 0.87       | 0.02        | 2         |
| A     | 10  | ILE  | HD11 | 0.014      | 0.02        | 1         |
| A     | 154 | ILE  | CG2  | 17.76      | 0.3         | 1         |
| A     | 160 | ASP  | N    | 116.396    | 0.3         | 1         |
| A     | 50  | THR  | HG23 | 0.996      | 0.02        | 1         |
| A     | 121 | GLY  | N    | 106.953    | 0.3         | 1         |
| A     | 67  | ASP  | C    | 172.107    | 0.3         | 1         |
| A     | 135 | THR  | CA   | 59.162     | 0.3         | 1         |
| A     | 83  | PRO  | HA   | 4.258      | 0.02        | 1         |
| A     | 118 | HIS  | HD2  | 6.589      | 0.02        | 1         |
| A     | 78  | ALA  | N    | 114.363    | 0.3         | 1         |
| A     | 26  | VAL  | CG1  | 21.225     | 0.3         | 1         |
| A     | 66  | ASP  | H    | 7.949      | 0.02        | 1         |
| A     | 19  | PRO  | HB3  | 1.97       | 0.02        | 2         |
| A     | 93  | PHE  | N    | 122.387    | 0.3         | 1         |
| A     | 133 | PHE  | HB3  | 3.097      | 0.02        | 2         |
| A     | 20  | ASP  | CG   | 178.21     | 0.3         | 1         |
| A     | 82  | GLY  | HA3  | 4.215      | 0.02        | 2         |
| A     | 102 | HIS  | C    | 173.225    | 0.3         | 1         |
| A     | 146 | LEU  | HD23 | 0.62       | 0.02        | 1         |
| A     | 137 | LYS  | HG2  | 1.13       | 0.02        | 1         |
| A     | 157 | LEU  | HB3  | 1.726      | 0.02        | 2         |
| A     | 28  | TYR  | HB2  | 3.188      | 0.02        | 2         |
| A     | 105 | GLY  | C    | 170.977    | 0.3         | 1         |
| A     | 100 | THR  | HA   | 4.807      | 0.02        | 1         |
| A     | 56  | LEU  | CA   | 50.569     | 0.3         | 1         |
| A     | 147 | SER  | HB3  | 3.777      | 0.02        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 67  | ASP  | CB   | 37.206     | 0.3         | 1         |
| A     | 20  | ASP  | H    | 8.739      | 0.02        | 1         |
| A     | 26  | VAL  | HG21 | 0.784      | 0.02        | 1         |
| A     | 54  | ASP  | N    | 121.373    | 0.3         | 1         |
| A     | 146 | LEU  | HB2  | 1.368      | 0.02        | 1         |
| A     | 13  | ARG  | CD   | 39.796     | 0.3         | 1         |
| A     | 116 | ILE  | CD1  | 9.301      | 0.3         | 1         |
| A     | 58  | VAL  | N    | 126.808    | 0.3         | 1         |
| A     | 106 | THR  | C    | 169.737    | 0.3         | 1         |
| A     | 35  | GLN  | CG   | 31.187     | 0.3         | 1         |
| A     | 40  | VAL  | HG13 | 0.807      | 0.02        | 1         |
| A     | 83  | PRO  | HD3  | 3.49       | 0.02        | 2         |
| A     | 61  | ARG  | N    | 118.113    | 0.3         | 1         |
| A     | 26  | VAL  | HG23 | 0.784      | 0.02        | 1         |
| A     | 158 | TYR  | HA   | 4.004      | 0.02        | 1         |
| A     | 35  | GLN  | C    | 175.057    | 0.3         | 1         |
| A     | 95  | GLU  | HA   | 4.784      | 0.02        | 1         |
| A     | 128 | PRO  | HD3  | 3.625      | 0.02        | 2         |
| A     | 16  | ASN  | HD22 | 6.887      | 0.02        | 1         |
| A     | 57  | VAL  | HG12 | 0.605      | 0.02        | 1         |
| A     | 55  | ILE  | CD1  | 11.616     | 0.3         | 1         |
| A     | 84  | GLY  | HA3  | 3.534      | 0.02        | 2         |
| A     | 85  | SER  | N    | 114.47     | 0.3         | 1         |
| A     | 29  | ALA  | HB2  | 1.386      | 0.02        | 1         |
| A     | 14  | ILE  | H    | 9.11       | 0.02        | 1         |
| A     | 37  | TRP  | N    | 116.762    | 0.3         | 1         |
| A     | 55  | ILE  | HG23 | 0.824      | 0.02        | 1         |
| A     | 81  | PHE  | H    | 11.91      | 0.02        | 1         |
| A     | 68  | HIS  | HA   | 4.524      | 0.02        | 1         |
| A     | 125 | SER  | HA   | 4.709      | 0.02        | 1         |
| A     | 76  | ILE  | HB   | 2.011      | 0.02        | 1         |
| A     | 153 | GLY  | H    | 8.269      | 0.02        | 1         |
| A     | 76  | ILE  | CB   | 35.314     | 0.3         | 1         |
| A     | 152 | ARG  | HA   | 3.991      | 0.02        | 1         |
| A     | 40  | VAL  | HG11 | 0.807      | 0.02        | 1         |
| A     | 40  | VAL  | N    | 105.538    | 0.3         | 1         |
| A     | 84  | GLY  | N    | 106.878    | 0.3         | 1         |
| A     | 90  | ASP  | CA   | 53.741     | 0.3         | 1         |
| A     | 150 | ASP  | HB3  | 2.722      | 0.02        | 2         |
| A     | 22  | ASN  | HD22 | 6.879      | 0.02        | 1         |
| A     | 116 | ILE  | HG23 | 0.064      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 54  | ASP  | HB2  | 2.869      | 0.02        | 1         |
| A     | 72  | GLY  | N    | 110.15     | 0.3         | 1         |
| A     | 117 | GLY  | C    | 174.779    | 0.3         | 1         |
| A     | 97  | GLU  | HB2  | 1.678      | 0.02        | 1         |
| A     | 58  | VAL  | CB   | 34.171     | 0.3         | 1         |
| A     | 18  | THR  | HG23 | 1.301      | 0.02        | 1         |
| A     | 22  | ASN  | CA   | 50.426     | 0.3         | 1         |
| A     | 121 | GLY  | CA   | 41.547     | 0.3         | 1         |
| A     | 61  | ARG  | HB2  | 1.545      | 0.02        | 1         |
| A     | 36  | VAL  | H    | 7.579      | 0.02        | 1         |
| A     | 122 | LEU  | CB   | 39.562     | 0.3         | 1         |
| A     | 85  | SER  | C    | 173.297    | 0.3         | 1         |
| A     | 142 | ASN  | CA   | 52.678     | 0.3         | 1         |
| A     | 144 | PHE  | HB3  | 2.772      | 0.02        | 2         |
| A     | 9   | TYR  | H    | 6.867      | 0.02        | 1         |
| A     | 48  | ILE  | H    | 8.683      | 0.02        | 1         |
| A     | 143 | THR  | HG23 | 0.999      | 0.02        | 1         |
| A     | 70  | PHE  | CB   | 36.0       | 0.3         | 1         |
| A     | 133 | PHE  | C    | 174.562    | 0.3         | 1         |
| A     | 140 | ASP  | HB3  | 2.627      | 0.02        | 2         |
| A     | 99  | TRP  | HB2  | 2.477      | 0.02        | 2         |
| A     | 137 | LYS  | CA   | 52.617     | 0.3         | 1         |
| A     | 12  | TYR  | HA   | 5.741      | 0.02        | 1         |
| A     | 33  | ALA  | HA   | 3.827      | 0.02        | 1         |
| A     | 151 | ILE  | HG22 | 0.759      | 0.02        | 1         |
| A     | 146 | LEU  | CD2  | 24.082     | 0.3         | 1         |
| A     | 113 | VAL  | HG21 | 0.012      | 0.02        | 1         |
| A     | 42  | PRO  | CA   | 60.612     | 0.3         | 1         |
| A     | 104 | GLY  | H    | 9.473      | 0.02        | 1         |
| A     | 129 | LYS  | CE   | 39.711     | 0.3         | 1         |
| A     | 21  | MET  | HA   | 4.477      | 0.02        | 1         |
| A     | 77  | LEU  | CA   | 52.773     | 0.3         | 1         |
| A     | 48  | ILE  | HG21 | 0.653      | 0.02        | 1         |
| A     | 119 | SER  | HB2  | 3.401      | 0.02        | 1         |
| A     | 10  | ILE  | CG2  | 14.085     | 0.3         | 1         |
| A     | 77  | LEU  | HD12 | -0.036     | 0.02        | 1         |
| A     | 154 | ILE  | HD13 | 0.757      | 0.02        | 1         |
| A     | 122 | LEU  | HB3  | 1.084      | 0.02        | 2         |
| A     | 101 | THR  | HG21 | 0.434      | 0.02        | 1         |
| A     | 54  | ASP  | CA   | 55.075     | 0.3         | 1         |
| A     | 79  | HIS  | HA   | 4.757      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 70  | PHE  | HA   | 4.829      | 0.02        | 1         |
| A     | 132 | MET  | HE2  | 0.364      | 0.02        | 1         |
| A     | 137 | LYS  | HD2  | 1.491      | 0.02        | 1         |
| A     | 80  | ALA  | N    | 122.807    | 0.3         | 1         |
| A     | 73  | LYS  | CE   | 39.307     | 0.3         | 1         |
| A     | 101 | THR  | H    | 7.908      | 0.02        | 1         |
| A     | 144 | PHE  | HA   | 4.01       | 0.02        | 1         |
| A     | 10  | ILE  | HA   | 4.04       | 0.02        | 1         |
| A     | 81  | PHE  | CB   | 38.59      | 0.3         | 1         |
| A     | 68  | HIS  | CB   | 27.631     | 0.3         | 1         |
| A     | 117 | GLY  | CA   | 45.442     | 0.3         | 1         |
| A     | 108 | LEU  | HD23 | -0.33      | 0.02        | 1         |
| A     | 129 | LYS  | H    | 8.151      | 0.02        | 1         |
| A     | 37  | TRP  | C    | 177.917    | 0.3         | 1         |
| A     | 69  | ALA  | HB2  | 1.189      | 0.02        | 1         |
| A     | 85  | SER  | CA   | 55.943     | 0.3         | 1         |
| A     | 63  | ALA  | CA   | 50.239     | 0.3         | 1         |
| A     | 96  | ASP  | HA   | 4.149      | 0.02        | 1         |
| A     | 87  | ILE  | CG1  | 25.333     | 0.3         | 1         |
| A     | 97  | GLU  | N    | 130.48     | 0.3         | 1         |
| A     | 44  | LYS  | C    | 173.352    | 0.3         | 1         |
| A     | 26  | VAL  | CA   | 64.009     | 0.3         | 1         |
| A     | 153 | GLY  | HA2  | 3.868      | 0.02        | 2         |
| A     | 145 | ARG  | N    | 126.185    | 0.3         | 1         |
| A     | 118 | HIS  | N    | 119.129    | 0.3         | 1         |
| A     | 122 | LEU  | H    | 8.289      | 0.02        | 1         |
| A     | 69  | ALA  | HB3  | 1.189      | 0.02        | 1         |
| A     | 110 | LEU  | HB3  | 1.448      | 0.02        | 2         |
| A     | 29  | ALA  | C    | 176.604    | 0.3         | 1         |
| A     | 40  | VAL  | CA   | 57.522     | 0.3         | 1         |
| A     | 123 | GLY  | HA2  | 4.316      | 0.02        | 2         |
| A     | 131 | VAL  | HG13 | 1.121      | 0.02        | 1         |
| A     | 83  | PRO  | C    | 171.928    | 0.3         | 1         |
| A     | 68  | HIS  | C    | 169.937    | 0.3         | 1         |
| A     | 65  | GLY  | N    | 108.634    | 0.3         | 1         |
| A     | 157 | LEU  | CD1  | 22.689     | 0.3         | 1         |
| A     | 148 | ALA  | CA   | 52.787     | 0.3         | 1         |
| A     | 70  | PHE  | H    | 7.92       | 0.02        | 1         |
| A     | 79  | HIS  | CA   | 51.16      | 0.3         | 1         |
| A     | 22  | ASN  | HA   | 4.537      | 0.02        | 1         |
| A     | 78  | ALA  | HA   | 4.778      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 89  | GLY  | N    | 119.477    | 0.3         | 1         |
| A     | 40  | VAL  | HG22 | 1.051      | 0.02        | 1         |
| A     | 36  | VAL  | N    | 116.949    | 0.3         | 1         |
| A     | 151 | ILE  | HD11 | 0.648      | 0.02        | 1         |
| A     | 116 | ILE  | H    | 8.806      | 0.02        | 1         |
| A     | 73  | LYS  | HA   | 3.469      | 0.02        | 1         |
| A     | 142 | ASN  | N    | 118.248    | 0.3         | 1         |
| A     | 43  | LEU  | HD13 | 0.594      | 0.02        | 1         |
| A     | 107 | ASN  | HD21 | 7.93       | 0.02        | 1         |
| A     | 93  | PHE  | CB   | 38.434     | 0.3         | 1         |
| A     | 17  | TYR  | HA   | 3.981      | 0.02        | 1         |
| A     | 137 | LYS  | N    | 129.709    | 0.3         | 1         |
| A     | 107 | ASN  | N    | 125.523    | 0.3         | 1         |
| A     | 35  | GLN  | NE2  | 112.879    | 0.3         | 1         |
| A     | 104 | GLY  | HA2  | 4.005      | 0.02        | 2         |
| A     | 28  | TYR  | C    | 173.49     | 0.3         | 1         |
| A     | 131 | VAL  | H    | 11.387     | 0.02        | 1         |
| A     | 46  | SER  | C    | 168.253    | 0.3         | 1         |
| A     | 68  | HIS  | H    | 7.446      | 0.02        | 1         |
| A     | 39  | ASN  | CA   | 52.229     | 0.3         | 1         |
| A     | 129 | LYS  | CB   | 29.213     | 0.3         | 1         |
| A     | 14  | ILE  | HG23 | -0.016     | 0.02        | 1         |
| A     | 59  | PHE  | HA   | 5.275      | 0.02        | 1         |
| A     | 130 | ALA  | N    | 123.681    | 0.3         | 1         |
| A     | 89  | GLY  | HA2  | 4.071      | 0.02        | 2         |
| A     | 93  | PHE  | HA   | 4.186      | 0.02        | 1         |
| A     | 169 | ASN  | HB3  | 2.56       | 0.02        | 2         |
| A     | 47  | LYS  | C    | 173.735    | 0.3         | 1         |
| A     | 148 | ALA  | C    | 177.381    | 0.3         | 1         |
| A     | 79  | HIS  | C    | 168.551    | 0.3         | 1         |
| A     | 34  | PHE  | N    | 113.9      | 0.3         | 1         |
| A     | 117 | GLY  | N    | 108.98     | 0.3         | 1         |
| A     | 132 | MET  | CB   | 24.407     | 0.3         | 1         |
| A     | 145 | ARG  | CA   | 51.352     | 0.3         | 1         |
| A     | 60  | ALA  | CA   | 48.363     | 0.3         | 1         |
| A     | 143 | THR  | CG2  | 18.57      | 0.3         | 1         |
| A     | 72  | GLY  | C    | 170.435    | 0.3         | 1         |
| A     | 58  | VAL  | HG23 | 0.791      | 0.02        | 1         |
| A     | 125 | SER  | H    | 6.729      | 0.02        | 1         |
| A     | 146 | LEU  | CG   | 28.996     | 0.3         | 1         |
| A     | 151 | ILE  | HG13 | 0.796      | 0.02        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 120 | LEU  | CD2  | 19.032     | 0.3         | 1         |
| A     | 117 | GLY  | HA3  | 2.234      | 0.02        | 2         |
| A     | 23  | ARG  | CB   | 26.961     | 0.3         | 1         |
| A     | 155 | GLN  | HE22 | 7.649      | 0.02        | 1         |
| A     | 76  | ILE  | N    | 129.153    | 0.3         | 1         |
| A     | 122 | LEU  | HD13 | 0.611      | 0.02        | 1         |
| A     | 64  | HIS  | H    | 7.794      | 0.02        | 1         |
| A     | 87  | ILE  | HG21 | 0.359      | 0.02        | 1         |
| A     | 14  | ILE  | CG2  | 13.861     | 0.3         | 1         |
| A     | 24  | GLU  | HB2  | 1.874      | 0.02        | 1         |
| A     | 89  | GLY  | CA   | 43.776     | 0.3         | 1         |
| A     | 13  | ARG  | HB2  | 1.496      | 0.02        | 1         |
| A     | 113 | VAL  | CA   | 65.574     | 0.3         | 1         |
| A     | 146 | LEU  | H    | 8.071      | 0.02        | 1         |
| A     | 139 | VAL  | CA   | 56.548     | 0.3         | 1         |
| A     | 154 | ILE  | HG12 | 1.471      | 0.02        | 2         |
| A     | 122 | LEU  | N    | 120.575    | 0.3         | 1         |
| A     | 149 | ASP  | HB3  | 2.395      | 0.02        | 2         |
| A     | 113 | VAL  | H    | 8.248      | 0.02        | 1         |
| A     | 91  | ALA  | HB1  | 0.905      | 0.02        | 1         |
| A     | 131 | VAL  | CG2  | 17.863     | 0.3         | 1         |
| A     | 12  | TYR  | HB2  | 2.861      | 0.02        | 2         |
| A     | 136 | TYR  | HB2  | 2.64       | 0.02        | 2         |
| A     | 36  | VAL  | CG1  | 20.036     | 0.3         | 1         |
| A     | 25  | ASP  | HB2  | 2.757      | 0.02        | 2         |
| A     | 29  | ALA  | HA   | 3.799      | 0.02        | 1         |
| A     | 77  | LEU  | HB2  | 1.317      | 0.02        | 1         |
| A     | 107 | ASN  | CA   | 52.769     | 0.3         | 1         |
| A     | 107 | ASN  | HB2  | 3.046      | 0.02        | 2         |
| A     | 128 | PRO  | HG2  | 1.609      | 0.02        | 2         |
| A     | 57  | VAL  | H    | 8.712      | 0.02        | 1         |
| A     | 120 | LEU  | HD11 | 0.206      | 0.02        | 1         |
| A     | 91  | ALA  | HA   | 4.6        | 0.02        | 1         |
| A     | 148 | ALA  | N    | 123.484    | 0.3         | 1         |
| A     | 137 | LYS  | HB3  | 1.545      | 0.02        | 2         |
| A     | 78  | ALA  | CA   | 48.606     | 0.3         | 1         |
| A     | 141 | ILE  | CG2  | 14.761     | 0.3         | 1         |
| A     | 109 | PHE  | N    | 119.852    | 0.3         | 1         |
| A     | 31  | ARG  | C    | 177.059    | 0.3         | 1         |
| A     | 26  | VAL  | HG11 | 0.875      | 0.02        | 1         |
| A     | 61  | ARG  | C    | 173.16     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 32  | LYS  | HG2  | 1.481      | 0.02        | 2         |
| A     | 33  | ALA  | CB   | 16.021     | 0.3         | 1         |
| A     | 139 | VAL  | HG12 | 0.729      | 0.02        | 1         |
| A     | 118 | HIS  | C    | 178.098    | 0.3         | 1         |
| A     | 13  | ARG  | CA   | 51.743     | 0.3         | 1         |
| A     | 35  | GLN  | CB   | 25.719     | 0.3         | 1         |
| A     | 19  | PRO  | HG2  | 1.8        | 0.02        | 2         |
| A     | 36  | VAL  | C    | 175.451    | 0.3         | 1         |
| A     | 11  | THR  | HG22 | 0.968      | 0.02        | 1         |
| A     | 116 | ILE  | HG21 | 0.064      | 0.02        | 1         |
| A     | 150 | ASP  | N    | 118.753    | 0.3         | 1         |
| A     | 148 | ALA  | HB3  | 1.348      | 0.02        | 1         |
| A     | 77  | LEU  | H    | 8.452      | 0.02        | 1         |
| A     | 27  | ASP  | H    | 8.3        | 0.02        | 1         |
| A     | 130 | ALA  | H    | 8.124      | 0.02        | 1         |
| A     | 154 | ILE  | C    | 175.368    | 0.3         | 1         |
| A     | 11  | THR  | CA   | 55.86      | 0.3         | 1         |
| A     | 80  | ALA  | HB3  | 1.156      | 0.02        | 1         |
| A     | 36  | VAL  | HG12 | 1.014      | 0.02        | 1         |
| A     | 20  | ASP  | HB2  | 2.582      | 0.02        | 2         |
| A     | 43  | LEU  | HD23 | 0.54       | 0.02        | 1         |
| A     | 71  | ASP  | CA   | 50.975     | 0.3         | 1         |
| A     | 168 | PRO  | CB   | 29.196     | 0.3         | 1         |
| A     | 149 | ASP  | CA   | 55.509     | 0.3         | 1         |
| A     | 108 | LEU  | CD2  | 19.105     | 0.3         | 1         |
| A     | 156 | SER  | CA   | 58.902     | 0.3         | 1         |
| A     | 76  | ILE  | CA   | 59.727     | 0.3         | 1         |
| A     | 138 | TYR  | C    | 172.175    | 0.3         | 1         |
| A     | 53  | ALA  | HB1  | 0.836      | 0.02        | 1         |
| A     | 22  | ASN  | HD21 | 7.551      | 0.02        | 1         |
| A     | 98  | PHE  | HA   | 4.688      | 0.02        | 1         |
| A     | 46  | SER  | N    | 116.544    | 0.3         | 1         |
| A     | 129 | LYS  | HA   | 4.002      | 0.02        | 1         |
| A     | 41  | THR  | HG21 | 1.379      | 0.02        | 1         |
| A     | 122 | LEU  | HD23 | 0.584      | 0.02        | 1         |
| A     | 88  | GLY  | C    | 171.663    | 0.3         | 1         |
| A     | 156 | SER  | CB   | 59.864     | 0.3         | 1         |
| A     | 27  | ASP  | C    | 176.864    | 0.3         | 1         |
| A     | 108 | LEU  | HB3  | 1.403      | 0.02        | 2         |
| A     | 143 | THR  | CB   | 66.707     | 0.3         | 1         |
| A     | 130 | ALA  | HB3  | 1.691      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 110 | LEU  | H    | 8.738      | 0.02        | 1         |
| A     | 142 | ASN  | CB   | 35.677     | 0.3         | 1         |
| A     | 92  | HIS  | N    | 121.186    | 0.3         | 1         |
| A     | 110 | LEU  | CD2  | 22.983     | 0.3         | 1         |
| A     | 32  | LYS  | C    | 175.953    | 0.3         | 1         |
| A     | 15  | ASN  | HB3  | 2.411      | 0.02        | 2         |
| A     | 33  | ALA  | H    | 7.948      | 0.02        | 1         |
| A     | 79  | HIS  | H    | 9.104      | 0.02        | 1         |
| A     | 159 | GLY  | N    | 109.424    | 0.3         | 1         |
| A     | 150 | ASP  | H    | 7.384      | 0.02        | 1         |
| A     | 41  | THR  | C    | 169.788    | 0.3         | 1         |
| A     | 32  | LYS  | CG   | 21.55      | 0.3         | 1         |
| A     | 35  | GLN  | H    | 8.04       | 0.02        | 1         |
| A     | 59  | PHE  | HB2  | 2.981      | 0.02        | 2         |
| A     | 11  | THR  | C    | 171.799    | 0.3         | 1         |
| A     | 21  | MET  | CG   | 29.118     | 0.3         | 1         |
| A     | 14  | ILE  | HD13 | 0.878      | 0.02        | 1         |
| A     | 143 | THR  | HG22 | 0.999      | 0.02        | 1         |
| A     | 30  | ILE  | HG22 | 0.64       | 0.02        | 1         |
| A     | 77  | LEU  | CB   | 41.185     | 0.3         | 1         |
| A     | 141 | ILE  | C    | 174.349    | 0.3         | 1         |
| A     | 140 | ASP  | CA   | 52.171     | 0.3         | 1         |
| A     | 27  | ASP  | CB   | 37.356     | 0.3         | 1         |
| A     | 130 | ALA  | CB   | 17.019     | 0.3         | 1         |
| A     | 157 | LEU  | HD23 | 0.532      | 0.02        | 1         |
| A     | 37  | TRP  | HB3  | 2.961      | 0.02        | 2         |
| A     | 129 | LYS  | HG3  | 1.254      | 0.02        | 2         |
| A     | 24  | GLU  | HA   | 4.023      | 0.02        | 1         |
| A     | 33  | ALA  | HB1  | 0.986      | 0.02        | 1         |
| A     | 25  | ASP  | CB   | 37.939     | 0.3         | 1         |
| A     | 21  | MET  | C    | 172.078    | 0.3         | 1         |
| A     | 142 | ASN  | HD22 | 7.904      | 0.02        | 1         |
| A     | 17  | TYR  | N    | 114.955    | 0.3         | 1         |
| A     | 52  | MET  | CB   | 29.079     | 0.3         | 1         |
| A     | 118 | HIS  | HA   | 4.677      | 0.02        | 1         |
| A     | 34  | PHE  | CB   | 35.926     | 0.3         | 1         |
| A     | 159 | GLY  | HA3  | 3.777      | 0.02        | 2         |
| A     | 116 | ILE  | HG13 | 0.184      | 0.02        | 2         |
| A     | 154 | ILE  | N    | 123.062    | 0.3         | 1         |
| A     | 88  | GLY  | CA   | 43.885     | 0.3         | 1         |
| A     | 103 | SER  | H    | 6.877      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 144 | PHE  | CA   | 57.134     | 0.3         | 1         |
| A     | 119 | SER  | H    | 8.593      | 0.02        | 1         |
| A     | 95  | GLU  | C    | 173.234    | 0.3         | 1         |
| A     | 65  | GLY  | H    | 7.675      | 0.02        | 1         |
| A     | 90  | ASP  | HA   | 4.085      | 0.02        | 1         |
| A     | 28  | TYR  | H    | 8.09       | 0.02        | 1         |
| A     | 156 | SER  | H    | 8.084      | 0.02        | 1         |
| A     | 145 | ARG  | HB3  | 1.309      | 0.02        | 2         |
| A     | 105 | GLY  | H    | 7.801      | 0.02        | 1         |
| A     | 16  | ASN  | H    | 7.718      | 0.02        | 1         |
| A     | 143 | THR  | H    | 7.545      | 0.02        | 1         |
| A     | 143 | THR  | HG21 | 0.999      | 0.02        | 1         |
| A     | 134 | PRO  | N    | 139.453    | 0.3         | 1         |
| A     | 9   | TYR  | CA   | 53.836     | 0.3         | 1         |
| A     | 35  | GLN  | HA   | 4.101      | 0.02        | 1         |
| A     | 43  | LEU  | CD1  | 20.207     | 0.3         | 1         |
| A     | 148 | ALA  | CB   | 14.997     | 0.3         | 1         |
| A     | 86  | GLY  | C    | 172.254    | 0.3         | 1         |
| A     | 79  | HIS  | CB   | 28.092     | 0.3         | 1         |
| A     | 141 | ILE  | CA   | 61.865     | 0.3         | 1         |
| A     | 24  | GLU  | CA   | 56.726     | 0.3         | 1         |
| A     | 98  | PHE  | C    | 174.583    | 0.3         | 1         |
| A     | 58  | VAL  | CG1  | 18.293     | 0.3         | 1         |
| A     | 40  | VAL  | HG21 | 1.051      | 0.02        | 1         |
| A     | 96  | ASP  | N    | 122.597    | 0.3         | 1         |
| A     | 68  | HIS  | HB3  | 2.471      | 0.02        | 2         |
| A     | 31  | ARG  | N    | 119.589    | 0.3         | 1         |
| A     | 158 | TYR  | H    | 7.608      | 0.02        | 1         |
| A     | 31  | ARG  | HG2  | 1.65       | 0.02        | 2         |
| A     | 43  | LEU  | HG   | 1.571      | 0.02        | 1         |
| A     | 92  | HIS  | CA   | 48.022     | 0.3         | 1         |
| A     | 58  | VAL  | HB   | 1.601      | 0.02        | 1         |
| A     | 12  | TYR  | N    | 117.274    | 0.3         | 1         |
| A     | 36  | VAL  | HG23 | 0.401      | 0.02        | 1         |
| A     | 31  | ARG  | HB2  | 1.958      | 0.02        | 2         |
| A     | 108 | LEU  | CB   | 38.199     | 0.3         | 1         |
| A     | 69  | ALA  | CB   | 15.391     | 0.3         | 1         |
| A     | 155 | GLN  | HG2  | 2.961      | 0.02        | 2         |
| A     | 56  | LEU  | HG   | 1.519      | 0.02        | 1         |
| A     | 108 | LEU  | HD12 | 0.65       | 0.02        | 1         |
| A     | 112 | ALA  | N    | 123.596    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 146 | LEU  | HD22 | 0.62       | 0.02        | 1         |
| A     | 106 | THR  | HB   | 2.355      | 0.02        | 1         |
| A     | 55  | ILE  | HG12 | 1.379      | 0.02        | 2         |
| A     | 154 | ILE  | HG23 | 1.455      | 0.02        | 1         |
| A     | 121 | GLY  | H    | 8.146      | 0.02        | 1         |
| A     | 122 | LEU  | HG   | 1.25       | 0.02        | 1         |
| A     | 124 | HIS  | CB   | 26.77      | 0.3         | 1         |
| A     | 104 | GLY  | HA3  | 3.714      | 0.02        | 2         |
| A     | 99  | TRP  | C    | 172.106    | 0.3         | 1         |
| A     | 129 | LYS  | CA   | 53.46      | 0.3         | 1         |
| A     | 126 | SER  | CA   | 55.809     | 0.3         | 1         |
| A     | 147 | SER  | N    | 117.994    | 0.3         | 1         |
| A     | 56  | LEU  | HA   | 4.965      | 0.02        | 1         |
| A     | 10  | ILE  | HG22 | 0.276      | 0.02        | 1         |
| A     | 33  | ALA  | N    | 123.489    | 0.3         | 1         |
| A     | 17  | TYR  | CA   | 55.977     | 0.3         | 1         |
| A     | 120 | LEU  | N    | 113.75     | 0.3         | 1         |
| A     | 156 | SER  | HB2  | 3.916      | 0.02        | 1         |
| A     | 21  | MET  | HE3  | 0.306      | 0.02        | 1         |
| A     | 16  | ASN  | HB2  | 2.939      | 0.02        | 2         |
| A     | 124 | HIS  | HB2  | 2.951      | 0.02        | 2         |
| A     | 24  | GLU  | C    | 176.605    | 0.3         | 1         |
| A     | 88  | GLY  | N    | 106.059    | 0.3         | 1         |
| A     | 73  | LYS  | CA   | 55.642     | 0.3         | 1         |
| A     | 52  | MET  | HG2  | 1.829      | 0.02        | 1         |
| A     | 92  | HIS  | HE1  | 9.175      | 0.02        | 1         |
| A     | 72  | GLY  | HA2  | 4.328      | 0.02        | 2         |
| A     | 152 | ARG  | HG3  | 1.496      | 0.02        | 2         |
| A     | 128 | PRO  | CD   | 47.953     | 0.3         | 1         |
| A     | 73  | LYS  | HE2  | 2.444      | 0.02        | 1         |
| A     | 5   | TRP  | N    | 122.976    | 0.3         | 1         |
| A     | 120 | LEU  | CD1  | 22.0       | 0.3         | 1         |
| A     | 143 | THR  | HB   | 4.232      | 0.02        | 1         |
| A     | 58  | VAL  | H    | 8.713      | 0.02        | 1         |
| A     | 88  | GLY  | HA3  | 2.959      | 0.02        | 2         |
| A     | 92  | HIS  | HD2  | 6.899      | 0.02        | 1         |
| A     | 158 | TYR  | HB2  | 3.097      | 0.02        | 1         |
| A     | 61  | ARG  | H    | 8.738      | 0.02        | 1         |
| A     | 30  | ILE  | HG13 | 0.966      | 0.02        | 2         |
| A     | 134 | PRO  | HA   | 3.745      | 0.02        | 1         |
| A     | 116 | ILE  | HD12 | -0.609     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 49  | ASN  | C    | 172.268    | 0.3         | 1         |
| A     | 57  | VAL  | HG23 | 0.852      | 0.02        | 1         |
| A     | 11  | THR  | H    | 9.097      | 0.02        | 1         |
| A     | 99  | TRP  | CA   | 50.853     | 0.3         | 1         |
| A     | 69  | ALA  | H    | 7.94       | 0.02        | 1         |
| A     | 56  | LEU  | HD21 | 1.012      | 0.02        | 1         |
| A     | 37  | TRP  | H    | 6.641      | 0.02        | 1         |
| A     | 115 | ALA  | CA   | 53.084     | 0.3         | 1         |
| A     | 156 | SER  | N    | 117.418    | 0.3         | 1         |
| A     | 39  | ASN  | N    | 114.792    | 0.3         | 1         |
| A     | 128 | PRO  | CB   | 29.1       | 0.3         | 1         |
| A     | 17  | TYR  | C    | 172.355    | 0.3         | 1         |
| A     | 157 | LEU  | HD11 | 0.629      | 0.02        | 1         |
| A     | 23  | ARG  | HD3  | 2.47       | 0.02        | 2         |
| A     | 73  | LYS  | HG2  | 1.468      | 0.02        | 2         |
| A     | 131 | VAL  | CG1  | 20.531     | 0.3         | 1         |
| A     | 144 | PHE  | N    | 123.197    | 0.3         | 1         |
| A     | 56  | LEU  | N    | 129.919    | 0.3         | 1         |
| A     | 52  | MET  | HA   | 4.36       | 0.02        | 1         |
| A     | 36  | VAL  | CG2  | 18.987     | 0.3         | 1         |
| A     | 107 | ASN  | ND2  | 111.286    | 0.3         | 1         |
| A     | 20  | ASP  | CA   | 53.31      | 0.3         | 1         |
| A     | 60  | ALA  | HB1  | 0.816      | 0.02        | 1         |
| A     | 55  | ILE  | HD12 | 0.996      | 0.02        | 1         |
| A     | 56  | LEU  | HD13 | 0.785      | 0.02        | 1         |
| A     | 112 | ALA  | CA   | 52.335     | 0.3         | 1         |
| A     | 142 | ASN  | HA   | 4.443      | 0.02        | 1         |
| A     | 120 | LEU  | HD12 | 0.206      | 0.02        | 1         |
| A     | 113 | VAL  | CG2  | 20.408     | 0.3         | 1         |
| A     | 47  | LYS  | CG   | 22.99      | 0.3         | 1         |
| A     | 141 | ILE  | CG1  | 24.352     | 0.3         | 1         |
| A     | 70  | PHE  | HB2  | 4.168      | 0.02        | 2         |
| A     | 126 | SER  | N    | 120.056    | 0.3         | 1         |
| A     | 135 | THR  | H    | 7.884      | 0.02        | 1         |
| A     | 105 | GLY  | HA3  | 3.829      | 0.02        | 2         |
| A     | 137 | LYS  | HA   | 3.9        | 0.02        | 1         |
| A     | 57  | VAL  | CG2  | 17.393     | 0.3         | 1         |
| A     | 13  | ARG  | CB   | 32.535     | 0.3         | 1         |
| A     | 94  | ASP  | N    | 120.718    | 0.3         | 1         |
| A     | 152 | ARG  | CA   | 56.494     | 0.3         | 1         |
| A     | 25  | ASP  | N    | 119.843    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 97  | GLU  | CB   | 28.562     | 0.3         | 1         |
| A     | 113 | VAL  | HG13 | 0.587      | 0.02        | 1         |
| A     | 110 | LEU  | HD11 | 0.421      | 0.02        | 1         |
| A     | 73  | LYS  | N    | 124.041    | 0.3         | 1         |
| A     | 56  | LEU  | C    | 172.963    | 0.3         | 1         |
| A     | 16  | ASN  | ND2  | 114.847    | 0.3         | 1         |
| A     | 61  | ARG  | CB   | 31.059     | 0.3         | 1         |
| A     | 107 | ASN  | H    | 8.498      | 0.02        | 1         |
| A     | 153 | GLY  | CA   | 44.637     | 0.3         | 1         |
| A     | 15  | ASN  | ND2  | 112.162    | 0.3         | 1         |
| A     | 143 | THR  | HA   | 4.281      | 0.02        | 1         |
| A     | 11  | THR  | CB   | 69.955     | 0.3         | 1         |
| A     | 38  | SER  | H    | 8.963      | 0.02        | 1         |
| A     | 4   | VAL  | HG11 | 0.416      | 0.02        | 1         |
| A     | 36  | VAL  | HB   | 1.972      | 0.02        | 1         |
| A     | 138 | TYR  | N    | 123.949    | 0.3         | 1         |
| A     | 31  | ARG  | HD2  | 3.178      | 0.02        | 1         |
| A     | 30  | ILE  | HD12 | 0.18       | 0.02        | 1         |
| A     | 71  | ASP  | CB   | 38.918     | 0.3         | 1         |
| A     | 20  | ASP  | C    | 173.123    | 0.3         | 1         |
| A     | 139 | VAL  | HA   | 3.789      | 0.02        | 1         |
| A     | 168 | PRO  | CA   | 60.173     | 0.3         | 1         |
| A     | 169 | ASN  | CB   | 35.859     | 0.3         | 1         |
| A     | 99  | TRP  | HE3  | 7.123      | 0.02        | 1         |
| A     | 127 | ASP  | HB3  | 2.316      | 0.02        | 2         |
| A     | 21  | MET  | HG2  | 2.208      | 0.02        | 2         |
| A     | 154 | ILE  | HB   | 2.053      | 0.02        | 1         |
| A     | 30  | ILE  | C    | 174.488    | 0.3         | 1         |
| A     | 35  | GLN  | HE21 | 7.533      | 0.02        | 1         |
| A     | 99  | TRP  | N    | 116.741    | 0.3         | 1         |
| A     | 110 | LEU  | HA   | 3.035      | 0.02        | 1         |
| A     | 76  | ILE  | HG23 | 1.164      | 0.02        | 1         |
| A     | 58  | VAL  | CA   | 58.098     | 0.3         | 1         |
| A     | 51  | GLY  | CA   | 41.364     | 0.3         | 1         |
| A     | 154 | ILE  | CG1  | 27.868     | 0.3         | 1         |
| A     | 96  | ASP  | CB   | 37.657     | 0.3         | 1         |
| A     | 113 | VAL  | HG12 | 0.587      | 0.02        | 1         |
| A     | 118 | HIS  | H    | 7.123      | 0.02        | 1         |
| A     | 50  | THR  | HG22 | 0.996      | 0.02        | 1         |
| A     | 42  | PRO  | HG2  | 1.505      | 0.02        | 1         |
| A     | 104 | GLY  | CA   | 42.184     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 119 | SER  | C    | 173.05     | 0.3         | 1         |
| A     | 135 | THR  | CB   | 69.073     | 0.3         | 1         |
| A     | 64  | HIS  | CA   | 54.639     | 0.3         | 1         |
| A     | 14  | ILE  | HG13 | 0.661      | 0.02        | 2         |
| A     | 19  | PRO  | HB2  | 2.129      | 0.02        | 2         |
| A     | 22  | ASN  | HB3  | 2.641      | 0.02        | 2         |
| A     | 82  | GLY  | HA2  | 4.34       | 0.02        | 2         |
| A     | 108 | LEU  | N    | 131.606    | 0.3         | 1         |
| A     | 49  | ASN  | CG   | 176.922    | 0.3         | 1         |
| A     | 139 | VAL  | H    | 5.727      | 0.02        | 1         |
| A     | 5   | TRP  | HE1  | 9.288      | 0.02        | 1         |
| A     | 148 | ALA  | H    | 8.77       | 0.02        | 1         |
| A     | 123 | GLY  | H    | 8.271      | 0.02        | 1         |
| A     | 30  | ILE  | HG21 | 0.64       | 0.02        | 1         |
| A     | 87  | ILE  | HD13 | 0.324      | 0.02        | 1         |
| A     | 140 | ASP  | CB   | 39.22      | 0.3         | 1         |
| A     | 124 | HIS  | N    | 115.595    | 0.3         | 1         |
| A     | 109 | PHE  | HA   | 3.795      | 0.02        | 1         |
| A     | 111 | THR  | H    | 7.283      | 0.02        | 1         |
| A     | 18  | THR  | H    | 8.09       | 0.02        | 1         |
| A     | 147 | SER  | HB2  | 4.099      | 0.02        | 2         |
| A     | 67  | ASP  | CA   | 52.652     | 0.3         | 1         |
| A     | 63  | ALA  | H    | 9.118      | 0.02        | 1         |
| A     | 33  | ALA  | HB2  | 0.986      | 0.02        | 1         |
| A     | 25  | ASP  | CA   | 54.232     | 0.3         | 1         |
| A     | 14  | ILE  | N    | 127.164    | 0.3         | 1         |
| A     | 26  | VAL  | H    | 7.683      | 0.02        | 1         |
| A     | 137 | LYS  | H    | 7.841      | 0.02        | 1         |
| A     | 52  | MET  | CA   | 52.309     | 0.3         | 1         |
| A     | 153 | GLY  | N    | 106.9      | 0.3         | 1         |
| A     | 81  | PHE  | N    | 131.38     | 0.3         | 1         |
| A     | 128 | PRO  | HD2  | 3.932      | 0.02        | 2         |
| A     | 77  | LEU  | CD2  | 18.824     | 0.3         | 1         |
| A     | 15  | ASN  | HA   | 4.207      | 0.02        | 1         |
| A     | 56  | LEU  | CD1  | 21.751     | 0.3         | 1         |
| A     | 57  | VAL  | HG13 | 0.605      | 0.02        | 1         |
| A     | 84  | GLY  | HA2  | 4.04       | 0.02        | 2         |
| A     | 19  | PRO  | CD   | 47.924     | 0.3         | 1         |
| A     | 76  | ILE  | CD1  | 9.716      | 0.3         | 1         |
| A     | 29  | ALA  | HB1  | 1.386      | 0.02        | 1         |
| A     | 132 | MET  | HA   | 4.497      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 116 | ILE  | C    | 174.612    | 0.3         | 1         |
| A     | 151 | ILE  | H    | 7.888      | 0.02        | 1         |
| A     | 96  | ASP  | H    | 8.161      | 0.02        | 1         |
| A     | 118 | HIS  | CB   | 25.289     | 0.3         | 1         |
| A     | 18  | THR  | C    | 170.997    | 0.3         | 1         |
| A     | 63  | ALA  | HB3  | 1.37       | 0.02        | 1         |
| A     | 48  | ILE  | CG1  | 23.295     | 0.3         | 1         |
| A     | 67  | ASP  | H    | 7.98       | 0.02        | 1         |
| A     | 13  | ARG  | HA   | 4.694      | 0.02        | 1         |
| A     | 44  | LYS  | CA   | 51.438     | 0.3         | 1         |
| A     | 137 | LYS  | HB2  | 1.472      | 0.02        | 2         |
| A     | 26  | VAL  | C    | 174.401    | 0.3         | 1         |
| A     | 51  | GLY  | HA2  | 4.306      | 0.02        | 2         |
| A     | 24  | GLU  | CB   | 25.74      | 0.3         | 1         |
| A     | 150 | ASP  | HB2  | 2.976      | 0.02        | 2         |
| A     | 58  | VAL  | CG2  | 17.999     | 0.3         | 1         |
| A     | 79  | HIS  | HD2  | 6.472      | 0.02        | 1         |
| A     | 116 | ILE  | HG22 | 0.064      | 0.02        | 1         |
| A     | 48  | ILE  | HG13 | 0.815      | 0.02        | 2         |
| A     | 141 | ILE  | HD11 | 0.598      | 0.02        | 1         |
| A     | 127 | ASP  | HA   | 4.62       | 0.02        | 1         |
| A     | 100 | THR  | N    | 126.21     | 0.3         | 1         |
| A     | 18  | THR  | HG22 | 1.301      | 0.02        | 1         |
| A     | 22  | ASN  | CB   | 35.26      | 0.3         | 1         |
| A     | 107 | ASN  | HA   | 4.715      | 0.02        | 1         |
| A     | 55  | ILE  | CA   | 58.738     | 0.3         | 1         |
| A     | 97  | GLU  | HA   | 4.349      | 0.02        | 1         |
| A     | 144 | PHE  | HB2  | 2.962      | 0.02        | 2         |
| A     | 147 | SER  | H    | 8.822      | 0.02        | 1         |
| A     | 94  | ASP  | C    | 173.832    | 0.3         | 1         |
| A     | 122 | LEU  | C    | 174.906    | 0.3         | 1         |
| A     | 135 | THR  | HG21 | 1.13       | 0.02        | 1         |
| A     | 61  | ARG  | HA   | 5.156      | 0.02        | 1         |
| A     | 30  | ILE  | HA   | 3.429      | 0.02        | 1         |
| A     | 82  | GLY  | CA   | 41.621     | 0.3         | 1         |
| A     | 69  | ALA  | CA   | 50.835     | 0.3         | 1         |
| A     | 96  | ASP  | HB3  | 2.588      | 0.02        | 2         |
| A     | 30  | ILE  | HD13 | 0.18       | 0.02        | 1         |
| A     | 111 | THR  | CG2  | 19.492     | 0.3         | 1         |
| A     | 80  | ALA  | H    | 8.589      | 0.02        | 1         |
| A     | 32  | LYS  | CD   | 25.0       | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 116 | ILE  | CG2  | 16.179     | 0.3         | 1         |
| A     | 146 | LEU  | CB   | 40.376     | 0.3         | 1         |
| A     | 137 | LYS  | CB   | 31.697     | 0.3         | 1         |
| A     | 50  | THR  | N    | 111.621    | 0.3         | 1         |
| A     | 101 | THR  | N    | 122.666    | 0.3         | 1         |
| A     | 151 | ILE  | HG23 | 0.759      | 0.02        | 1         |
| A     | 43  | LEU  | CG   | 26.192     | 0.3         | 1         |
| A     | 86  | GLY  | HA3  | 3.627      | 0.02        | 2         |
| A     | 129 | LYS  | CD   | 26.216     | 0.3         | 1         |
| A     | 102 | HIS  | HB2  | 3.136      | 0.02        | 2         |
| A     | 48  | ILE  | HG22 | 0.653      | 0.02        | 1         |
| A     | 4   | VAL  | HB   | 1.215      | 0.02        | 1         |
| A     | 87  | ILE  | HA   | 4.13       | 0.02        | 1         |
| A     | 67  | ASP  | HB2  | 2.952      | 0.02        | 1         |
| A     | 10  | ILE  | CG1  | 25.467     | 0.3         | 1         |
| A     | 77  | LEU  | HD13 | -0.036     | 0.02        | 1         |
| A     | 154 | ILE  | HD12 | 0.757      | 0.02        | 1         |
| A     | 141 | ILE  | HA   | 3.703      | 0.02        | 1         |
| A     | 109 | PHE  | C    | 172.747    | 0.3         | 1         |
| A     | 46  | SER  | HA   | 4.522      | 0.02        | 1         |
| A     | 114 | HIS  | H    | 6.874      | 0.02        | 1         |
| A     | 132 | MET  | HE3  | 0.364      | 0.02        | 1         |
| A     | 81  | PHE  | C    | 172.848    | 0.3         | 1         |
| A     | 41  | THR  | HA   | 5.168      | 0.02        | 1         |
| A     | 64  | HIS  | HA   | 4.702      | 0.02        | 1         |
| A     | 123 | GLY  | N    | 109.69     | 0.3         | 1         |
| A     | 84  | GLY  | C    | 168.95     | 0.3         | 1         |
| A     | 10  | ILE  | HG12 | 0.654      | 0.02        | 2         |
| A     | 4   | VAL  | CG1  | 24.761     | 0.3         | 1         |
| A     | 10  | ILE  | HB   | 1.25       | 0.02        | 1         |
| A     | 145 | ARG  | CB   | 30.566     | 0.3         | 1         |
| A     | 120 | LEU  | HD22 | 0.732      | 0.02        | 1         |
| A     | 75  | GLY  | HA3  | 3.305      | 0.02        | 2         |
| A     | 92  | HIS  | HA   | 5.695      | 0.02        | 1         |
| A     | 118 | HIS  | HB3  | 2.353      | 0.02        | 2         |
| A     | 132 | MET  | N    | 115.3      | 0.3         | 1         |
| A     | 93  | PHE  | C    | 170.893    | 0.3         | 1         |
| A     | 42  | PRO  | C    | 172.744    | 0.3         | 1         |
| A     | 59  | PHE  | H    | 8.296      | 0.02        | 1         |
| A     | 69  | ALA  | HB1  | 1.189      | 0.02        | 1         |
| A     | 151 | ILE  | HD13 | 0.648      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 138 | TYR  | HB2  | 2.923      | 0.02        | 2         |
| A     | 113 | VAL  | C    | 175.735    | 0.3         | 1         |
| A     | 109 | PHE  | HD1  | 6.555      | 0.02        | 3         |
| A     | 48  | ILE  | C    | 172.186    | 0.3         | 1         |
| A     | 120 | LEU  | HA   | 4.224      | 0.02        | 1         |
| A     | 110 | LEU  | HB2  | 1.682      | 0.02        | 2         |
| A     | 144 | PHE  | H    | 7.162      | 0.02        | 1         |
| A     | 60  | ALA  | H    | 9.049      | 0.02        | 1         |
| A     | 123 | GLY  | HA3  | 3.511      | 0.02        | 2         |
| A     | 34  | PHE  | C    | 175.936    | 0.3         | 1         |
| A     | 58  | VAL  | HG11 | 0.626      | 0.02        | 1         |
| A     | 106 | THR  | H    | 9.101      | 0.02        | 1         |
| A     | 76  | ILE  | HD13 | 0.903      | 0.02        | 1         |
| A     | 74  | GLY  | N    | 121.103    | 0.3         | 1         |
| A     | 99  | TRP  | CB   | 23.024     | 0.3         | 1         |
| A     | 152 | ARG  | CG   | 24.38      | 0.3         | 1         |
| A     | 66  | ASP  | C    | 170.985    | 0.3         | 1         |
| A     | 50  | THR  | H    | 7.384      | 0.02        | 1         |
| A     | 100 | THR  | HG23 | 0.939      | 0.02        | 1         |
| A     | 103 | SER  | HB2  | 3.078      | 0.02        | 1         |
| A     | 11  | THR  | HB   | 3.977      | 0.02        | 1         |
| A     | 87  | ILE  | H    | 8.938      | 0.02        | 1         |
| A     | 155 | GLN  | C    | 177.321    | 0.3         | 1         |
| A     | 11  | THR  | CG2  | 19.124     | 0.3         | 1         |
| A     | 55  | ILE  | N    | 124.32     | 0.3         | 1         |
| A     | 106 | THR  | HG21 | 0.203      | 0.02        | 1         |
| A     | 122 | LEU  | HD12 | 0.611      | 0.02        | 1         |
| A     | 43  | LEU  | HD12 | 0.594      | 0.02        | 1         |
| A     | 157 | LEU  | CA   | 53.831     | 0.3         | 1         |
| A     | 60  | ALA  | HB2  | 0.816      | 0.02        | 1         |
| A     | 82  | GLY  | N    | 105.239    | 0.3         | 1         |
| A     | 111 | THR  | HG21 | 1.254      | 0.02        | 1         |
| A     | 90  | ASP  | H    | 8.265      | 0.02        | 1         |
| A     | 93  | PHE  | CA   | 54.121     | 0.3         | 1         |
| A     | 40  | VAL  | C    | 171.526    | 0.3         | 1         |
| A     | 83  | PRO  | CA   | 61.327     | 0.3         | 1         |
| A     | 45  | PHE  | CA   | 52.812     | 0.3         | 1         |
| A     | 32  | LYS  | N    | 118.961    | 0.3         | 1         |
| A     | 160 | ASP  | H    | 7.879      | 0.02        | 1         |
| A     | 113 | VAL  | CG1  | 21.065     | 0.3         | 1         |
| A     | 147 | SER  | HA   | 4.418      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 112 | ALA  | HB3  | 0.953      | 0.02        | 1         |
| A     | 141 | ILE  | CB   | 34.827     | 0.3         | 1         |
| A     | 61  | ARG  | HG2  | 1.294      | 0.02        | 1         |
| A     | 117 | GLY  | H    | 7.604      | 0.02        | 1         |
| A     | 136 | TYR  | CA   | 56.066     | 0.3         | 1         |
| A     | 39  | ASN  | CB   | 36.206     | 0.3         | 1         |
| A     | 50  | THR  | C    | 169.819    | 0.3         | 1         |
| A     | 14  | ILE  | HG22 | -0.016     | 0.02        | 1         |
| A     | 57  | VAL  | CG1  | 18.025     | 0.3         | 1         |
| A     | 48  | ILE  | CA   | 56.182     | 0.3         | 1         |
| A     | 15  | ASN  | C    | 171.058    | 0.3         | 1         |
| A     | 71  | ASP  | HB2  | 3.009      | 0.02        | 2         |
| A     | 58  | VAL  | C    | 171.925    | 0.3         | 1         |
| A     | 89  | GLY  | HA3  | 3.665      | 0.02        | 2         |
| A     | 77  | LEU  | HD23 | 0.181      | 0.02        | 1         |
| A     | 48  | ILE  | HD11 | 0.541      | 0.02        | 1         |
| A     | 39  | ASN  | HD22 | 6.917      | 0.02        | 1         |
| A     | 79  | HIS  | HB2  | 3.219      | 0.02        | 2         |
| A     | 97  | GLU  | CG   | 32.661     | 0.3         | 1         |
| A     | 123 | GLY  | CA   | 40.113     | 0.3         | 1         |
| A     | 35  | GLN  | N    | 118.904    | 0.3         | 1         |
| A     | 160 | ASP  | HB2  | 2.615      | 0.02        | 2         |
| A     | 115 | ALA  | HB1  | 1.06       | 0.02        | 1         |
| A     | 61  | ARG  | CA   | 51.021     | 0.3         | 1         |
| A     | 132 | MET  | CA   | 50.715     | 0.3         | 1         |
| A     | 13  | ARG  | C    | 171.433    | 0.3         | 1         |
| A     | 60  | ALA  | CB   | 20.011     | 0.3         | 1         |
| A     | 99  | TRP  | H    | 7.319      | 0.02        | 1         |
| A     | 107 | ASN  | HD22 | 6.255      | 0.02        | 1         |
| A     | 50  | THR  | CB   | 68.127     | 0.3         | 1         |
| A     | 36  | VAL  | CA   | 63.266     | 0.3         | 1         |
| A     | 17  | TYR  | H    | 8.537      | 0.02        | 1         |
| A     | 139 | VAL  | HB   | 1.754      | 0.02        | 1         |
| A     | 23  | ARG  | CD   | 40.427     | 0.3         | 1         |
| A     | 168 | PRO  | CD   | 46.964     | 0.3         | 1         |
| A     | 151 | ILE  | HG12 | 1.67       | 0.02        | 2         |
| A     | 117 | GLY  | HA2  | 3.768      | 0.02        | 2         |
| A     | 95  | GLU  | HB2  | 1.986      | 0.02        | 2         |
| A     | 47  | LYS  | HD2  | 1.65       | 0.02        | 1         |
| A     | 23  | ARG  | CA   | 57.689     | 0.3         | 1         |
| A     | 44  | LYS  | HG2  | 1.297      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 100 | THR  | HG21 | 0.939      | 0.02        | 1         |
| A     | 95  | GLU  | HG3  | 2.097      | 0.02        | 2         |
| A     | 14  | ILE  | CG1  | 25.155     | 0.3         | 1         |
| A     | 136 | TYR  | C    | 171.319    | 0.3         | 1         |
| A     | 134 | PRO  | C    | 171.414    | 0.3         | 1         |
| A     | 77  | LEU  | HA   | 4.374      | 0.02        | 1         |
| A     | 15  | ASN  | HD22 | 7.021      | 0.02        | 1         |
| A     | 4   | VAL  | CA   | 59.78      | 0.3         | 1         |
| A     | 105 | GLY  | N    | 108.27     | 0.3         | 1         |
| A     | 72  | GLY  | CA   | 40.898     | 0.3         | 1         |
| A     | 15  | ASN  | CA   | 53.577     | 0.3         | 1         |
| A     | 17  | TYR  | HB3  | 2.482      | 0.02        | 2         |
| A     | 31  | ARG  | CG   | 24.141     | 0.3         | 1         |
| A     | 50  | THR  | HG21 | 0.996      | 0.02        | 1         |
| A     | 154 | ILE  | HG13 | 1.457      | 0.02        | 2         |
| A     | 48  | ILE  | CD1  | 9.75       | 0.3         | 1         |
| A     | 143 | THR  | N    | 109.5      | 0.3         | 1         |
| A     | 149 | ASP  | HB2  | 2.719      | 0.02        | 2         |
| A     | 157 | LEU  | N    | 118.102    | 0.3         | 1         |
| A     | 44  | LYS  | H    | 8.119      | 0.02        | 1         |
| A     | 12  | TYR  | HB3  | 2.23       | 0.02        | 2         |
| A     | 136 | TYR  | HB3  | 2.17       | 0.02        | 2         |
| A     | 6   | ARG  | CB   | 27.705     | 0.3         | 1         |
| A     | 83  | PRO  | N    | 133.221    | 0.3         | 1         |
| A     | 49  | ASN  | CB   | 37.074     | 0.3         | 1         |
| A     | 31  | ARG  | HB3  | 1.882      | 0.02        | 2         |
| A     | 46  | SER  | HB2  | 3.422      | 0.02        | 2         |
| A     | 136 | TYR  | N    | 127.452    | 0.3         | 1         |
| A     | 159 | GLY  | CA   | 41.313     | 0.3         | 1         |
| A     | 65  | GLY  | C    | 172.207    | 0.3         | 1         |
| A     | 77  | LEU  | N    | 127.756    | 0.3         | 1         |
| A     | 56  | LEU  | CG   | 24.39      | 0.3         | 1         |
| A     | 155 | GLN  | HA   | 4.189      | 0.02        | 1         |
| A     | 56  | LEU  | HB3  | 1.328      | 0.02        | 2         |
| A     | 27  | ASP  | N    | 118.287    | 0.3         | 1         |
| A     | 32  | LYS  | HG3  | 1.408      | 0.02        | 2         |
| A     | 82  | GLY  | H    | 8.163      | 0.02        | 1         |
| A     | 139 | VAL  | HG13 | 0.729      | 0.02        | 1         |
| A     | 6   | ARG  | HA   | 4.423      | 0.02        | 1         |
| A     | 74  | GLY  | C    | 171.413    | 0.3         | 1         |
| A     | 141 | ILE  | HG12 | 1.051      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 120 | LEU  | CG   | 23.209     | 0.3         | 1         |
| A     | 155 | GLN  | HB3  | 2.197      | 0.02        | 2         |
| A     | 35  | GLN  | CA   | 55.576     | 0.3         | 1         |
| A     | 33  | ALA  | C    | 175.821    | 0.3         | 1         |
| A     | 157 | LEU  | HA   | 4.036      | 0.02        | 1         |
| A     | 19  | PRO  | HG3  | 1.716      | 0.02        | 2         |
| A     | 11  | THR  | HG23 | 0.968      | 0.02        | 1         |
| A     | 154 | ILE  | CB   | 35.774     | 0.3         | 1         |
| A     | 144 | PHE  | CB   | 36.701     | 0.3         | 1         |
| A     | 58  | VAL  | HA   | 4.856      | 0.02        | 1         |
| A     | 77  | LEU  | CD1  | 21.201     | 0.3         | 1         |
| A     | 56  | LEU  | CD2  | 21.216     | 0.3         | 1         |
| A     | 141 | ILE  | H    | 7.777      | 0.02        | 1         |
| A     | 157 | LEU  | CB   | 40.492     | 0.3         | 1         |
| A     | 46  | SER  | H    | 7.975      | 0.02        | 1         |
| A     | 36  | VAL  | HG11 | 1.014      | 0.02        | 1         |
| A     | 20  | ASP  | HB3  | 2.403      | 0.02        | 2         |
| A     | 35  | GLN  | HG2  | 2.446      | 0.02        | 2         |
| A     | 51  | GLY  | H    | 8.207      | 0.02        | 1         |
| A     | 19  | PRO  | C    | 174.321    | 0.3         | 1         |
| A     | 151 | ILE  | HB   | 1.62       | 0.02        | 1         |
| A     | 108 | LEU  | CD1  | 24.797     | 0.3         | 1         |
| A     | 118 | HIS  | CA   | 54.974     | 0.3         | 1         |
| A     | 158 | TYR  | CA   | 56.804     | 0.3         | 1         |
| A     | 14  | ILE  | HG12 | 1.609      | 0.02        | 2         |
| A     | 5   | TRP  | C    | 172.235    | 0.3         | 1         |
| A     | 90  | ASP  | C    | 170.711    | 0.3         | 1         |
| A     | 92  | HIS  | H    | 9.018      | 0.02        | 1         |
| A     | 145 | ARG  | HG2  | 1.36       | 0.02        | 2         |
| A     | 44  | LYS  | CB   | 38.3       | 0.3         | 1         |
| A     | 146 | LEU  | HG   | 1.32       | 0.02        | 1         |
| A     | 147 | SER  | CB   | 63.168     | 0.3         | 1         |
| A     | 53  | ALA  | HB2  | 0.836      | 0.02        | 1         |
| A     | 65  | GLY  | CA   | 42.867     | 0.3         | 1         |
| A     | 4   | VAL  | N    | 110.21     | 0.3         | 1         |
| A     | 79  | HIS  | N    | 113.788    | 0.3         | 1         |
| A     | 15  | ASN  | N    | 128.561    | 0.3         | 1         |
| A     | 56  | LEU  | HD11 | 0.785      | 0.02        | 1         |
| A     | 122 | LEU  | HD22 | 0.584      | 0.02        | 1         |
| A     | 52  | MET  | HB2  | 2.406      | 0.02        | 1         |
| A     | 22  | ASN  | HB2  | 2.728      | 0.02        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 142 | ASN  | C    | 173.703    | 0.3         | 1         |
| A     | 18  | THR  | HG21 | 1.301      | 0.02        | 1         |
| A     | 128 | PRO  | HB3  | 1.385      | 0.02        | 2         |
| A     | 143 | THR  | CA   | 58.367     | 0.3         | 1         |
| A     | 130 | ALA  | HB2  | 1.691      | 0.02        | 1         |
| A     | 101 | THR  | C    | 171.412    | 0.3         | 1         |
| A     | 80  | ALA  | HA   | 4.134      | 0.02        | 1         |
| A     | 92  | HIS  | HB3  | 2.356      | 0.02        | 2         |
| A     | 135 | THR  | HG22 | 1.13       | 0.02        | 1         |
| A     | 30  | ILE  | HB   | 2.035      | 0.02        | 1         |
| A     | 137 | LYS  | C    | 170.759    | 0.3         | 1         |
| A     | 114 | HIS  | HA   | 4.244      | 0.02        | 1         |
| A     | 83  | PRO  | HB2  | 2.123      | 0.02        | 2         |
| A     | 53  | ALA  | H    | 7.904      | 0.02        | 1         |
| A     | 38  | SER  | HB3  | 4.073      | 0.02        | 2         |
| A     | 152 | ARG  | H    | 8.484      | 0.02        | 1         |
| A     | 69  | ALA  | HA   | 4.511      | 0.02        | 1         |
| A     | 116 | ILE  | CG1  | 26.482     | 0.3         | 1         |
| A     | 137 | LYS  | CG   | 21.203     | 0.3         | 1         |
| A     | 77  | LEU  | C    | 173.288    | 0.3         | 1         |
| A     | 139 | VAL  | HG23 | 0.675      | 0.02        | 1         |
| A     | 42  | PRO  | CG   | 24.247     | 0.3         | 1         |
| A     | 47  | LYS  | N    | 127.558    | 0.3         | 1         |
| A     | 122 | LEU  | HA   | 4.398      | 0.02        | 1         |
| A     | 14  | ILE  | HD12 | 0.878      | 0.02        | 1         |
| A     | 114 | HIS  | CA   | 56.08      | 0.3         | 1         |
| A     | 64  | HIS  | HB2  | 4.095      | 0.02        | 2         |
| A     | 99  | TRP  | HB3  | 1.777      | 0.02        | 2         |
| A     | 124 | HIS  | HA   | 4.953      | 0.02        | 1         |
| A     | 154 | ILE  | H    | 8.587      | 0.02        | 1         |
| A     | 4   | VAL  | HA   | 4.392      | 0.02        | 1         |
| A     | 27  | ASP  | CA   | 55.161     | 0.3         | 1         |
| A     | 6   | ARG  | HB2  | 1.837      | 0.02        | 1         |
| A     | 154 | ILE  | HD11 | 0.757      | 0.02        | 1         |
| A     | 141 | ILE  | HB   | 1.768      | 0.02        | 1         |
| A     | 130 | ALA  | CA   | 48.997     | 0.3         | 1         |
| A     | 85  | SER  | H    | 8.293      | 0.02        | 1         |
| A     | 65  | GLY  | HA2  | 3.713      | 0.02        | 2         |
| A     | 76  | ILE  | HG12 | 1.628      | 0.02        | 2         |
| A     | 152 | ARG  | HD2  | 3.124      | 0.02        | 1         |
| A     | 131 | VAL  | N    | 130.727    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 4   | VAL  | CG2  | 24.152     | 0.3         | 1         |
| A     | 68  | HIS  | HD2  | 6.444      | 0.02        | 1         |
| A     | 141 | ILE  | CD1  | 10.725     | 0.3         | 1         |
| A     | 159 | GLY  | HA2  | 4.208      | 0.02        | 2         |
| A     | 16  | ASN  | HA   | 4.58       | 0.02        | 1         |
| A     | 115 | ALA  | HA   | 4.017      | 0.02        | 1         |
| A     | 126 | SER  | H    | 8.764      | 0.02        | 1         |
| A     | 60  | ALA  | N    | 125.759    | 0.3         | 1         |
| A     | 122 | LEU  | CD2  | 20.325     | 0.3         | 1         |
| A     | 94  | ASP  | H    | 7.912      | 0.02        | 1         |
| A     | 155 | GLN  | NE2  | 117.198    | 0.3         | 1         |
| A     | 145 | ARG  | HB2  | 1.542      | 0.02        | 2         |
| A     | 31  | ARG  | H    | 8.2        | 0.02        | 1         |
| A     | 109 | PHE  | HD2  | 6.836      | 0.02        | 3         |
| A     | 116 | ILE  | HA   | 3.432      | 0.02        | 1         |
| A     | 95  | GLU  | N    | 120.958    | 0.3         | 1         |
| A     | 73  | LYS  | H    | 8.668      | 0.02        | 1         |
| A     | 86  | GLY  | CA   | 44.259     | 0.3         | 1         |
| A     | 131 | VAL  | HG11 | 1.121      | 0.02        | 1         |
| A     | 71  | ASP  | HA   | 4.825      | 0.02        | 1         |
| A     | 151 | ILE  | CA   | 63.079     | 0.3         | 1         |
| A     | 169 | ASN  | HA   | 4.775      | 0.02        | 1         |
| A     | 129 | LYS  | N    | 116.552    | 0.3         | 1         |
| A     | 146 | LEU  | HD11 | 1.166      | 0.02        | 1         |
| A     | 112 | ALA  | H    | 9.132      | 0.02        | 1         |
| A     | 35  | GLN  | HB2  | 2.158      | 0.02        | 1         |
| A     | 130 | ALA  | C    | 176.866    | 0.3         | 1         |
| A     | 134 | PRO  | HB2  | 1.924      | 0.02        | 1         |
| A     | 27  | ASP  | HB3  | 2.585      | 0.02        | 2         |
| A     | 142 | ASN  | HB2  | 2.819      | 0.02        | 2         |
| A     | 122 | LEU  | CG   | 23.564     | 0.3         | 1         |
| A     | 76  | ILE  | H    | 10.567     | 0.02        | 1         |
| A     | 22  | ASN  | C    | 174.513    | 0.3         | 1         |
| A     | 78  | ALA  | HB3  | 1.003      | 0.02        | 1         |
| A     | 45  | PHE  | CB   | 39.011     | 0.3         | 1         |
| A     | 49  | ASN  | N    | 119.411    | 0.3         | 1         |
| A     | 155 | GLN  | HG3  | 2.913      | 0.02        | 2         |
| A     | 108 | LEU  | HD13 | 0.65       | 0.02        | 1         |
| A     | 115 | ALA  | H    | 8.639      | 0.02        | 1         |
| A     | 39  | ASN  | C    | 174.066    | 0.3         | 1         |
| A     | 106 | THR  | HA   | 3.581      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 98  | PHE  | CA   | 53.991     | 0.3         | 1         |
| A     | 154 | ILE  | HG22 | 1.455      | 0.02        | 1         |
| A     | 145 | ARG  | HD3  | 2.931      | 0.02        | 2         |
| A     | 110 | LEU  | HD21 | 0.691      | 0.02        | 1         |
| A     | 88  | GLY  | H    | 7.576      | 0.02        | 1         |
| A     | 110 | LEU  | CG   | 23.361     | 0.3         | 1         |
| A     | 126 | SER  | CB   | 61.315     | 0.3         | 1         |
| A     | 91  | ALA  | CA   | 48.137     | 0.3         | 1         |
| A     | 48  | ILE  | CB   | 37.688     | 0.3         | 1         |
| A     | 10  | ILE  | HG21 | 0.276      | 0.02        | 1         |
| A     | 124 | HIS  | C    | 172.617    | 0.3         | 1         |
| A     | 101 | THR  | HA   | 4.544      | 0.02        | 1         |
| A     | 92  | HIS  | C    | 169.965    | 0.3         | 1         |
| A     | 48  | ILE  | HD12 | 0.541      | 0.02        | 1         |
| A     | 39  | ASN  | HD21 | 7.524      | 0.02        | 1         |
| A     | 5   | TRP  | H    | 7.929      | 0.02        | 1         |
| A     | 13  | ARG  | N    | 118.851    | 0.3         | 1         |
| A     | 99  | TRP  | NE1  | 126.897    | 0.3         | 1         |
| A     | 97  | GLU  | CD   | 180.485    | 0.3         | 1         |
| A     | 124 | HIS  | HB3  | 2.803      | 0.02        | 2         |
| A     | 115 | ALA  | HB2  | 1.06       | 0.02        | 1         |
| A     | 121 | GLY  | HA2  | 4.063      | 0.02        | 2         |
| A     | 73  | LYS  | HD2  | 1.522      | 0.02        | 1         |
| A     | 100 | THR  | CG2  | 17.802     | 0.3         | 1         |
| A     | 45  | PHE  | HB2  | 2.402      | 0.02        | 2         |
| A     | 108 | LEU  | H    | 8.41       | 0.02        | 1         |
| A     | 66  | ASP  | HB2  | 2.786      | 0.02        | 2         |
| A     | 72  | GLY  | HA3  | 4.169      | 0.02        | 2         |
| A     | 102 | HIS  | H    | 7.498      | 0.02        | 1         |
| A     | 11  | THR  | N    | 117.229    | 0.3         | 1         |
| A     | 146 | LEU  | CA   | 51.999     | 0.3         | 1         |
| A     | 74  | GLY  | HA2  | 4.111      | 0.02        | 2         |
| A     | 71  | ASP  | N    | 116.247    | 0.3         | 1         |
| A     | 88  | GLY  | HA2  | 3.665      | 0.02        | 2         |
| A     | 169 | ASN  | N    | 119.792    | 0.3         | 1         |
| A     | 100 | THR  | HG22 | 0.939      | 0.02        | 1         |
| A     | 116 | ILE  | HD11 | -0.609     | 0.02        | 1         |
| A     | 122 | LEU  | HD11 | 0.611      | 0.02        | 1         |
| A     | 151 | ILE  | N    | 118.9      | 0.3         | 1         |
| A     | 32  | LYS  | HD2  | 0.861      | 0.02        | 2         |
| A     | 48  | ILE  | HB   | 1.81       | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 57  | VAL  | HG22 | 0.852      | 0.02        | 1         |
| A     | 87  | ILE  | HG23 | 0.359      | 0.02        | 1         |
| A     | 103 | SER  | C    | 173.13     | 0.3         | 1         |
| A     | 140 | ASP  | HA   | 4.139      | 0.02        | 1         |
| A     | 45  | PHE  | H    | 8.109      | 0.02        | 1         |
| A     | 42  | PRO  | HD2  | 2.88       | 0.02        | 1         |
| A     | 56  | LEU  | HD22 | 1.012      | 0.02        | 1         |
| A     | 91  | ALA  | C    | 171.694    | 0.3         | 1         |
| A     | 15  | ASN  | CB   | 38.873     | 0.3         | 1         |
| A     | 115 | ALA  | CB   | 15.398     | 0.3         | 1         |
| A     | 113 | VAL  | HG11 | 0.587      | 0.02        | 1         |
| A     | 111 | THR  | HB   | 4.223      | 0.02        | 1         |
| A     | 16  | ASN  | CG   | 175.137    | 0.3         | 1         |
| A     | 95  | GLU  | H    | 8.007      | 0.02        | 1         |
| A     | 100 | THR  | C    | 172.185    | 0.3         | 1         |
| A     | 157 | LEU  | HD21 | 0.532      | 0.02        | 1         |
| A     | 157 | LEU  | HD12 | 0.629      | 0.02        | 1         |
| A     | 91  | ALA  | HB3  | 0.905      | 0.02        | 1         |
| A     | 55  | ILE  | CG2  | 12.079     | 0.3         | 1         |
| A     | 120 | LEU  | C    | 175.22     | 0.3         | 1         |
| A     | 20  | ASP  | CB   | 39.097     | 0.3         | 1         |
| A     | 129 | LYS  | HB2  | 1.689      | 0.02        | 1         |
| A     | 55  | ILE  | HD13 | 0.996      | 0.02        | 1         |
| A     | 49  | ASN  | CA   | 50.628     | 0.3         | 1         |
| A     | 56  | LEU  | HD12 | 0.785      | 0.02        | 1         |
| A     | 108 | LEU  | HG   | 0.968      | 0.02        | 1         |
| A     | 62  | GLY  | CA   | 43.728     | 0.3         | 1         |
| A     | 14  | ILE  | HA   | 4.217      | 0.02        | 1         |
| A     | 78  | ALA  | C    | 173.574    | 0.3         | 1         |
| A     | 120 | LEU  | HD13 | 0.206      | 0.02        | 1         |
| A     | 73  | LYS  | CB   | 29.28      | 0.3         | 1         |
| A     | 21  | MET  | N    | 113.047    | 0.3         | 1         |
| A     | 86  | GLY  | N    | 112.395    | 0.3         | 1         |
| A     | 70  | PHE  | HB3  | 3.105      | 0.02        | 2         |
| A     | 9   | TYR  | HB3  | 2.608      | 0.02        | 2         |
| A     | 140 | ASP  | N    | 119.172    | 0.3         | 1         |
| A     | 79  | HIS  | HE1  | 8.032      | 0.02        | 1         |
| A     | 38  | SER  | N    | 117.922    | 0.3         | 1         |
| A     | 32  | LYS  | HA   | 3.802      | 0.02        | 1         |
| A     | 101 | THR  | HG22 | 0.434      | 0.02        | 1         |
| A     | 109 | PHE  | HE1  | 7.171      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 112 | ALA  | HA   | 3.989      | 0.02        | 1         |
| A     | 44  | LYS  | HA   | 4.335      | 0.02        | 1         |
| A     | 146 | LEU  | CD1  | 28.215     | 0.3         | 1         |
| A     | 14  | ILE  | CB   | 33.524     | 0.3         | 1         |
| A     | 40  | VAL  | HA   | 4.684      | 0.02        | 1         |
| A     | 109 | PHE  | HB2  | 3.315      | 0.02        | 2         |
| A     | 131 | VAL  | CB   | 28.285     | 0.3         | 1         |
| A     | 148 | ALA  | HB1  | 1.348      | 0.02        | 1         |
| A     | 154 | ILE  | CA   | 58.219     | 0.3         | 1         |
| A     | 108 | LEU  | HD22 | -0.33      | 0.02        | 1         |
| A     | 131 | VAL  | HG23 | 0.934      | 0.02        | 1         |
| A     | 71  | ASP  | C    | 174.565    | 0.3         | 1         |
| A     | 80  | ALA  | HB1  | 1.156      | 0.02        | 1         |
| A     | 152 | ARG  | C    | 177.87     | 0.3         | 1         |
| A     | 30  | ILE  | HD11 | 0.18       | 0.02        | 1         |
| A     | 15  | ASN  | H    | 9.604      | 0.02        | 1         |
| A     | 145 | ARG  | CD   | 40.602     | 0.3         | 1         |
| A     | 169 | ASN  | CA   | 48.443     | 0.3         | 1         |
| A     | 148 | ALA  | HA   | 3.957      | 0.02        | 1         |
| A     | 95  | GLU  | CB   | 26.431     | 0.3         | 1         |
| A     | 127 | ASP  | HB2  | 2.911      | 0.02        | 2         |
| A     | 132 | MET  | H    | 7.541      | 0.02        | 1         |
| A     | 103 | SER  | N    | 115.418    | 0.3         | 1         |
| A     | 141 | ILE  | HG23 | 0.923      | 0.02        | 1         |
| A     | 51  | GLY  | HA3  | 3.998      | 0.02        | 2         |
| A     | 129 | LYS  | HD3  | 1.562      | 0.02        | 2         |
| A     | 135 | THR  | CG2  | 19.149     | 0.3         | 1         |
| A     | 24  | GLU  | N    | 116.093    | 0.3         | 1         |
| A     | 12  | TYR  | C    | 169.021    | 0.3         | 1         |
| A     | 41  | THR  | HG23 | 1.379      | 0.02        | 1         |
| A     | 122 | LEU  | HD21 | 0.584      | 0.02        | 1         |
| A     | 57  | VAL  | N    | 125.516    | 0.3         | 1         |
| A     | 76  | ILE  | HG22 | 1.164      | 0.02        | 1         |
| A     | 128 | PRO  | CG   | 24.21      | 0.3         | 1         |
| A     | 10  | ILE  | HD13 | 0.014      | 0.02        | 1         |
| A     | 135 | THR  | C    | 170.456    | 0.3         | 1         |
| A     | 96  | ASP  | CA   | 51.205     | 0.3         | 1         |
| A     | 23  | ARG  | H    | 8.902      | 0.02        | 1         |
| A     | 130 | ALA  | HB1  | 1.691      | 0.02        | 1         |
| A     | 45  | PHE  | HA   | 5.582      | 0.02        | 1         |
| A     | 98  | PHE  | HB2  | 2.451      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 62  | GLY  | N    | 108.004    | 0.3         | 1         |
| A     | 25  | ASP  | HA   | 4.555      | 0.02        | 1         |
| A     | 137 | LYS  | CD   | 26.187     | 0.3         | 1         |
| A     | 146 | LEU  | HD21 | 0.62       | 0.02        | 1         |
| A     | 72  | GLY  | H    | 8.792      | 0.02        | 1         |
| A     | 61  | ARG  | HD2  | 3.165      | 0.02        | 1         |
| A     | 87  | ILE  | N    | 134.118    | 0.3         | 1         |
| A     | 140 | ASP  | C    | 176.195    | 0.3         | 1         |
| A     | 76  | ILE  | CG2  | 15.732     | 0.3         | 1         |
| A     | 14  | ILE  | HD11 | 0.878      | 0.02        | 1         |
| A     | 159 | GLY  | H    | 8.299      | 0.02        | 1         |
| A     | 87  | ILE  | HD12 | 0.324      | 0.02        | 1         |
| A     | 127 | ASP  | N    | 126.571    | 0.3         | 1         |
| A     | 23  | ARG  | HB3  | 1.234      | 0.02        | 2         |
| A     | 147 | SER  | CA   | 54.845     | 0.3         | 1         |
| A     | 62  | GLY  | HA3  | 3.657      | 0.02        | 2         |
| A     | 119 | SER  | CA   | 60.246     | 0.3         | 1         |
| A     | 19  | PRO  | HD3  | 3.488      | 0.02        | 2         |
| A     | 33  | ALA  | HB3  | 0.986      | 0.02        | 1         |
| A     | 47  | LYS  | HB3  | 0.994      | 0.02        | 2         |
| A     | 32  | LYS  | H    | 8.462      | 0.02        | 1         |
| A     | 102 | HIS  | HA   | 4.712      | 0.02        | 1         |
| A     | 145 | ARG  | HA   | 3.872      | 0.02        | 1         |
| A     | 132 | MET  | HB3  | 1.692      | 0.02        | 2         |
| A     | 19  | PRO  | CG   | 24.249     | 0.3         | 1         |
| A     | 55  | ILE  | HG21 | 0.824      | 0.02        | 1         |
| A     | 116 | ILE  | HB   | 1.284      | 0.02        | 1         |
| A     | 116 | ILE  | CB   | 34.496     | 0.3         | 1         |
| A     | 63  | ALA  | HB2  | 1.37       | 0.02        | 1         |
| A     | 48  | ILE  | CG2  | 14.284     | 0.3         | 1         |
| A     | 47  | LYS  | HG2  | 0.799      | 0.02        | 1         |
| A     | 32  | LYS  | HB2  | 1.439      | 0.02        | 1         |
| A     | 23  | ARG  | N    | 125.97     | 0.3         | 1         |
| A     | 146 | LEU  | HD12 | 1.166      | 0.02        | 1         |
| A     | 93  | PHE  | H    | 8.971      | 0.02        | 1         |
| A     | 48  | ILE  | HG12 | 0.989      | 0.02        | 2         |
| A     | 60  | ALA  | HA   | 4.754      | 0.02        | 1         |
| A     | 160 | ASP  | CA   | 48.436     | 0.3         | 1         |
| A     | 115 | ALA  | N    | 120.337    | 0.3         | 1         |
| A     | 126 | SER  | HB2  | 4.093      | 0.02        | 2         |
| A     | 145 | ARG  | H    | 7.112      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 43  | LEU  | HA   | 4.334      | 0.02        | 1         |
| A     | 30  | ILE  | CG2  | 15.987     | 0.3         | 1         |
| A     | 55  | ILE  | CB   | 37.326     | 0.3         | 1         |
| A     | 87  | ILE  | HG12 | 0.875      | 0.02        | 2         |
| A     | 125 | SER  | C    | 172.66     | 0.3         | 1         |
| A     | 18  | THR  | CA   | 55.892     | 0.3         | 1         |
| A     | 20  | ASP  | N    | 121.788    | 0.3         | 1         |
| A     | 128 | PRO  | HB2  | 1.713      | 0.02        | 2         |
| A     | 96  | ASP  | HB2  | 2.702      | 0.02        | 2         |
| A     | 32  | LYS  | CB   | 27.967     | 0.3         | 1         |
| A     | 129 | LYS  | C    | 174.023    | 0.3         | 1         |
| A     | 49  | ASN  | H    | 8.727      | 0.02        | 1         |
| A     | 157 | LEU  | C    | 175.397    | 0.3         | 1         |
| A     | 113 | VAL  | HG23 | 0.012      | 0.02        | 1         |
| A     | 42  | PRO  | HB2  | 1.559      | 0.02        | 1         |
| A     | 21  | MET  | CB   | 36.413     | 0.3         | 1         |
| A     | 110 | LEU  | HD22 | 0.691      | 0.02        | 1         |
| A     | 110 | LEU  | CB   | 40.146     | 0.3         | 1         |
| A     | 142 | ASN  | H    | 8.452      | 0.02        | 1         |
| A     | 86  | GLY  | HA2  | 3.894      | 0.02        | 2         |
| A     | 129 | LYS  | CG   | 21.943     | 0.3         | 1         |
| A     | 102 | HIS  | HB3  | 2.697      | 0.02        | 2         |
| A     | 77  | LEU  | CG   | 23.227     | 0.3         | 1         |
| A     | 48  | ILE  | HG23 | 0.653      | 0.02        | 1         |
| A     | 133 | PHE  | N    | 128.151    | 0.3         | 1         |
| A     | 87  | ILE  | HB   | 1.37       | 0.02        | 1         |
| A     | 45  | PHE  | C    | 173.785    | 0.3         | 1         |
| A     | 119 | SER  | N    | 122.583    | 0.3         | 1         |
| A     | 41  | THR  | CG2  | 21.848     | 0.3         | 1         |
| A     | 55  | ILE  | C    | 170.451    | 0.3         | 1         |
| A     | 125 | SER  | CB   | 62.609     | 0.3         | 1         |
| A     | 94  | ASP  | CA   | 55.648     | 0.3         | 1         |
| A     | 21  | MET  | HE1  | 0.306      | 0.02        | 1         |
| A     | 41  | THR  | HB   | 3.983      | 0.02        | 1         |
| A     | 29  | ALA  | CB   | 15.638     | 0.3         | 1         |
| A     | 73  | LYS  | CG   | 21.871     | 0.3         | 1         |
| A     | 142 | ASN  | HD21 | 6.956      | 0.02        | 1         |
| A     | 10  | ILE  | HG13 | 0.1        | 0.02        | 2         |
| A     | 138 | TYR  | CB   | 35.556     | 0.3         | 1         |
| A     | 136 | TYR  | H    | 8.973      | 0.02        | 1         |
| A     | 75  | GLY  | HA2  | 3.92       | 0.02        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 118 | HIS  | HB2  | 3.627      | 0.02        | 2         |
| A     | 39  | ASN  | HA   | 4.557      | 0.02        | 1         |
| A     | 10  | ILE  | C    | 172.521    | 0.3         | 1         |
| A     | 111 | THR  | CA   | 63.87      | 0.3         | 1         |
| A     | 15  | ASN  | HD21 | 7.946      | 0.02        | 1         |
| A     | 118 | HIS  | HE1  | 8.373      | 0.02        | 1         |
| A     | 13  | ARG  | HG2  | 1.462      | 0.02        | 1         |
| A     | 141 | ILE  | N    | 124.692    | 0.3         | 1         |
| A     | 141 | ILE  | HD12 | 0.598      | 0.02        | 1         |
| A     | 25  | ASP  | H    | 7.409      | 0.02        | 1         |
| A     | 39  | ASN  | ND2  | 111.562    | 0.3         | 1         |
| A     | 138 | TYR  | HB3  | 2.605      | 0.02        | 2         |
| A     | 37  | TRP  | CA   | 55.625     | 0.3         | 1         |
| A     | 63  | ALA  | C    | 174.207    | 0.3         | 1         |
| A     | 52  | MET  | H    | 8.181      | 0.02        | 1         |
| A     | 113 | VAL  | CB   | 28.258     | 0.3         | 1         |
| A     | 103 | SER  | CB   | 60.76      | 0.3         | 1         |
| A     | 85  | SER  | HB3  | 3.835      | 0.02        | 2         |
| A     | 55  | ILE  | H    | 8.785      | 0.02        | 1         |
| A     | 57  | VAL  | HG21 | 0.852      | 0.02        | 1         |
| A     | 84  | GLY  | CA   | 41.277     | 0.3         | 1         |
| A     | 80  | ALA  | C    | 177.15     | 0.3         | 1         |
| A     | 115 | ALA  | C    | 176.179    | 0.3         | 1         |
| A     | 28  | TYR  | CB   | 35.942     | 0.3         | 1         |
| A     | 155 | GLN  | CG   | 32.087     | 0.3         | 1         |
| A     | 57  | VAL  | CB   | 29.83      | 0.3         | 1         |
| A     | 155 | GLN  | CB   | 23.892     | 0.3         | 1         |
| A     | 51  | GLY  | N    | 109.896    | 0.3         | 1         |
| A     | 16  | ASN  | CB   | 35.78      | 0.3         | 1         |
| A     | 11  | THR  | HA   | 5.24       | 0.02        | 1         |
| A     | 108 | LEU  | C    | 173.484    | 0.3         | 1         |
| A     | 21  | MET  | H    | 6.811      | 0.02        | 1         |
| A     | 136 | TYR  | HA   | 4.567      | 0.02        | 1         |
| A     | 104 | GLY  | N    | 115.132    | 0.3         | 1         |
| A     | 106 | THR  | HG22 | 0.203      | 0.02        | 1         |
| A     | 43  | LEU  | HD11 | 0.594      | 0.02        | 1         |
| A     | 49  | ASN  | ND2  | 109.786    | 0.3         | 1         |
| A     | 114 | HIS  | HB2  | 3.788      | 0.02        | 2         |
| A     | 4   | VAL  | C    | 172.708    | 0.3         | 1         |
| A     | 60  | ALA  | HB3  | 0.816      | 0.02        | 1         |
| A     | 64  | HIS  | N    | 124.847    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 111 | THR  | HG22 | 1.254      | 0.02        | 1         |
| A     | 39  | ASN  | HB2  | 2.905      | 0.02        | 2         |
| A     | 6   | ARG  | N    | 115.526    | 0.3         | 1         |
| A     | 108 | LEU  | CG   | 25.05      | 0.3         | 1         |
| A     | 83  | PRO  | CB   | 28.9       | 0.3         | 1         |
| A     | 38  | SER  | C    | 173.046    | 0.3         | 1         |
| A     | 27  | ASP  | HA   | 4.249      | 0.02        | 1         |
| A     | 112 | ALA  | HB2  | 0.953      | 0.02        | 1         |
| A     | 29  | ALA  | H    | 7.984      | 0.02        | 1         |
| A     | 42  | PRO  | N    | 128.123    | 0.3         | 1         |
| A     | 47  | LYS  | CE   | 40.16      | 0.3         | 1         |
| A     | 130 | ALA  | HA   | 4.459      | 0.02        | 1         |
| A     | 125 | SER  | HB3  | 3.362      | 0.02        | 2         |
| A     | 26  | VAL  | HG12 | 0.875      | 0.02        | 1         |
| A     | 136 | TYR  | CB   | 36.108     | 0.3         | 1         |
| A     | 127 | ASP  | CB   | 39.163     | 0.3         | 1         |
| A     | 135 | THR  | N    | 116.478    | 0.3         | 1         |
| A     | 14  | ILE  | HG21 | -0.016     | 0.02        | 1         |
| A     | 23  | ARG  | HD2  | 2.55       | 0.02        | 2         |
| A     | 71  | ASP  | HB3  | 2.476      | 0.02        | 2         |
| A     | 77  | LEU  | HD22 | 0.181      | 0.02        | 1         |
| A     | 21  | MET  | HB3  | 1.273      | 0.02        | 2         |
| A     | 14  | ILE  | CA   | 58.6       | 0.3         | 1         |
| A     | 80  | ALA  | CA   | 47.825     | 0.3         | 1         |
| A     | 40  | VAL  | HB   | 2.576      | 0.02        | 1         |
| A     | 153 | GLY  | C    | 174.279    | 0.3         | 1         |
| A     | 30  | ILE  | CB   | 32.607     | 0.3         | 1         |
| A     | 110 | LEU  | HD13 | 0.421      | 0.02        | 1         |
| A     | 160 | ASP  | HB3  | 2.529      | 0.02        | 2         |
| A     | 6   | ARG  | C    | 177.138    | 0.3         | 1         |
| A     | 108 | LEU  | HD21 | -0.33      | 0.02        | 1         |
| A     | 111 | THR  | N    | 112.535    | 0.3         | 1         |
| A     | 63  | ALA  | N    | 134.082    | 0.3         | 1         |
| A     | 58  | VAL  | HG21 | 0.791      | 0.02        | 1         |
| A     | 4   | VAL  | HG13 | 0.416      | 0.02        | 1         |
| A     | 49  | ASN  | HD21 | 6.672      | 0.02        | 1         |
| A     | 50  | THR  | CA   | 57.521     | 0.3         | 1         |
| A     | 36  | VAL  | CB   | 28.204     | 0.3         | 1         |
| A     | 26  | VAL  | N    | 123.993    | 0.3         | 1         |
| A     | 57  | VAL  | HA   | 5.07       | 0.02        | 1         |
| A     | 155 | GLN  | H    | 8.652      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 168 | PRO  | CG   | 24.288     | 0.3         | 1         |
| A     | 145 | ARG  | CG   | 22.997     | 0.3         | 1         |
| A     | 99  | TRP  | HE1  | 10.109     | 0.02        | 1         |
| A     | 95  | GLU  | HB3  | 1.85       | 0.02        | 2         |
| A     | 137 | LYS  | HE2  | 2.801      | 0.02        | 1         |
| A     | 131 | VAL  | HA   | 4.291      | 0.02        | 1         |
| A     | 15  | ASN  | HB2  | 2.999      | 0.02        | 2         |
| A     | 31  | ARG  | HG3  | 1.492      | 0.02        | 2         |
| A     | 123 | GLY  | C    | 170.905    | 0.3         | 1         |
| A     | 157 | LEU  | H    | 6.749      | 0.02        | 1         |
| A     | 102 | HIS  | CA   | 50.934     | 0.3         | 1         |
| A     | 95  | GLU  | HG2  | 2.208      | 0.02        | 2         |
| A     | 44  | LYS  | N    | 122.655    | 0.3         | 1         |
| A     | 26  | VAL  | HG13 | 0.875      | 0.02        | 1         |
| A     | 150 | ASP  | CB   | 41.541     | 0.3         | 1         |
| A     | 152 | ARG  | HB3  | 1.792      | 0.02        | 2         |
| A     | 5   | TRP  | HA   | 4.982      | 0.02        | 1         |
| A     | 4   | VAL  | CB   | 38.285     | 0.3         | 1         |
| A     | 23  | ARG  | HG2  | 0.917      | 0.02        | 2         |
| A     | 104 | GLY  | C    | 170.841    | 0.3         | 1         |
| A     | 17  | TYR  | HB2  | 2.721      | 0.02        | 2         |
| A     | 31  | ARG  | CD   | 41.111     | 0.3         | 1         |
| A     | 14  | ILE  | C    | 172.315    | 0.3         | 1         |
| A     | 127 | ASP  | H    | 8.848      | 0.02        | 1         |
| A     | 49  | ASN  | HB2  | 2.778      | 0.02        | 1         |
| A     | 151 | ILE  | CD1  | 10.325     | 0.3         | 1         |
| A     | 106 | THR  | CA   | 59.841     | 0.3         | 1         |
| A     | 6   | ARG  | CA   | 51.629     | 0.3         | 1         |
| A     | 10  | ILE  | CD1  | 10.099     | 0.3         | 1         |
| A     | 75  | GLY  | H    | 8.417      | 0.02        | 1         |
| A     | 30  | ILE  | H    | 7.983      | 0.02        | 1         |
| A     | 157 | LEU  | HB2  | 1.777      | 0.02        | 2         |
| A     | 137 | LYS  | CE   | 39.436     | 0.3         | 1         |
| A     | 34  | PHE  | H    | 7.649      | 0.02        | 1         |
| A     | 97  | GLU  | HG2  | 2.505      | 0.02        | 1         |
| A     | 46  | SER  | HB3  | 3.314      | 0.02        | 2         |
| A     | 87  | ILE  | HD11 | 0.324      | 0.02        | 1         |
| A     | 47  | LYS  | CB   | 30.468     | 0.3         | 1         |
| A     | 43  | LEU  | N    | 111.126    | 0.3         | 1         |
| A     | 56  | LEU  | HB2  | 1.566      | 0.02        | 2         |
| A     | 119 | SER  | CB   | 60.549     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 52  | MET  | C    | 172.201    | 0.3         | 1         |
| A     | 108 | LEU  | HA   | 4.315      | 0.02        | 1         |
| A     | 13  | ARG  | CG   | 26.116     | 0.3         | 1         |
| A     | 155 | GLN  | HB2  | 2.097      | 0.02        | 2         |
| A     | 40  | VAL  | HG12 | 0.807      | 0.02        | 1         |
| A     | 83  | PRO  | HD2  | 3.673      | 0.02        | 2         |
| A     | 29  | ALA  | N    | 121.412    | 0.3         | 1         |
| A     | 28  | TYR  | HB3  | 2.985      | 0.02        | 2         |
| A     | 26  | VAL  | HA   | 3.402      | 0.02        | 1         |
| A     | 90  | ASP  | HB2  | 2.888      | 0.02        | 1         |
| A     | 25  | ASP  | C    | 176.396    | 0.3         | 1         |
| A     | 16  | ASN  | HD21 | 7.821      | 0.02        | 1         |
| A     | 57  | VAL  | HG11 | 0.605      | 0.02        | 1         |
| A     | 31  | ARG  | HA   | 4.002      | 0.02        | 1         |
| A     | 128 | PRO  | N    | 136.982    | 0.3         | 1         |
| A     | 19  | PRO  | CB   | 28.839     | 0.3         | 1         |
| A     | 29  | ALA  | HB3  | 1.386      | 0.02        | 1         |
| A     | 121 | GLY  | C    | 171.493    | 0.3         | 1         |
| A     | 4   | VAL  | H    | 8.229      | 0.02        | 1         |
| A     | 35  | GLN  | HG3  | 2.33       | 0.02        | 2         |
| A     | 151 | ILE  | CG2  | 14.021     | 0.3         | 1         |
| A     | 43  | LEU  | HD21 | 0.54       | 0.02        | 1         |
| A     | 55  | ILE  | HG22 | 0.824      | 0.02        | 1         |
| A     | 158 | TYR  | CB   | 38.603     | 0.3         | 1         |
| A     | 63  | ALA  | HB1  | 1.37       | 0.02        | 1         |
| A     | 76  | ILE  | HA   | 3.823      | 0.02        | 1         |
| A     | 94  | ASP  | HA   | 4.086      | 0.02        | 1         |
| A     | 145 | ARG  | HG3  | 1.29       | 0.02        | 2         |
| A     | 102 | HIS  | N    | 120.547    | 0.3         | 1         |
| A     | 149 | ASP  | C    | 175.908    | 0.3         | 1         |
| A     | 41  | THR  | CB   | 69.444     | 0.3         | 1         |
| A     | 53  | ALA  | HB3  | 0.836      | 0.02        | 1         |
| A     | 138 | TYR  | HA   | 3.647      | 0.02        | 1         |
| A     | 67  | ASP  | HA   | 4.321      | 0.02        | 1         |
| A     | 28  | TYR  | N    | 119.607    | 0.3         | 1         |
| A     | 141 | ILE  | HD13 | 0.598      | 0.02        | 1         |
| A     | 139 | VAL  | N    | 124.19     | 0.3         | 1         |
| A     | 71  | ASP  | H    | 8.218      | 0.02        | 1         |
| A     | 155 | GLN  | N    | 123.4      | 0.3         | 1         |
| A     | 23  | ARG  | HB2  | 1.345      | 0.02        | 2         |
| A     | 169 | ASN  | H    | 8.381      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 114 | HIS  | C    | 172.67     | 0.3         | 1         |
| A     | 16  | ASN  | N    | 113.007    | 0.3         | 1         |
| A     | 114 | HIS  | HB3  | 2.982      | 0.02        | 2         |
| A     | 151 | ILE  | C    | 174.834    | 0.3         | 1         |
| A     | 10  | ILE  | H    | 8.194      | 0.02        | 1         |
| A     | 122 | LEU  | CA   | 52.311     | 0.3         | 1         |
| A     | 47  | LYS  | H    | 8.057      | 0.02        | 1         |
| A     | 124 | HIS  | H    | 8.353      | 0.02        | 1         |
| A     | 49  | ASN  | HA   | 4.74       | 0.02        | 1         |
| A     | 54  | ASP  | C    | 174.181    | 0.3         | 1         |
| A     | 82  | GLY  | C    | 168.147    | 0.3         | 1         |
| A     | 106 | THR  | N    | 124.763    | 0.3         | 1         |
| A     | 92  | HIS  | HB2  | 3.048      | 0.02        | 2         |
| A     | 135 | THR  | HG23 | 1.13       | 0.02        | 1         |
| A     | 74  | GLY  | H    | 10.689     | 0.02        | 1         |
| A     | 83  | PRO  | HB3  | 1.711      | 0.02        | 2         |
| A     | 140 | ASP  | HB2  | 2.912      | 0.02        | 2         |
| A     | 38  | SER  | HB2  | 4.258      | 0.02        | 2         |
| A     | 133 | PHE  | HB2  | 3.537      | 0.02        | 2         |
| A     | 45  | PHE  | N    | 119.696    | 0.3         | 1         |
| A     | 32  | LYS  | CA   | 55.402     | 0.3         | 1         |
| A     | 30  | ILE  | CD1  | 5.65       | 0.3         | 1         |
| A     | 139 | VAL  | HG22 | 0.675      | 0.02        | 1         |
| A     | 56  | LEU  | CB   | 40.78      | 0.3         | 1         |
| A     | 37  | TRP  | HE1  | 10.027     | 0.02        | 1         |
| A     | 43  | LEU  | CA   | 56.586     | 0.3         | 1         |
| A     | 64  | HIS  | HB3  | 3.377      | 0.02        | 2         |
| A     | 109 | PHE  | CA   | 58.876     | 0.3         | 1         |
| A     | 155 | GLN  | HE21 | 8.256      | 0.02        | 1         |
| A     | 143 | THR  | C    | 171.121    | 0.3         | 1         |
| A     | 122 | LEU  | HB2  | 1.402      | 0.02        | 2         |
| A     | 16  | ASN  | C    | 167.039    | 0.3         | 1         |
| A     | 48  | ILE  | N    | 123.812    | 0.3         | 1         |
| A     | 65  | GLY  | HA3  | 3.991      | 0.02        | 2         |
| A     | 113 | VAL  | HA   | 3.083      | 0.02        | 1         |
| A     | 138 | TYR  | H    | 8.5        | 0.02        | 1         |
| A     | 97  | GLU  | C    | 173.785    | 0.3         | 1         |
| A     | 132 | MET  | HE1  | 0.364      | 0.02        | 1         |
| A     | 76  | ILE  | HG13 | 1.295      | 0.02        | 2         |
| A     | 29  | ALA  | CA   | 52.892     | 0.3         | 1         |
| A     | 87  | ILE  | CD1  | 11.492     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 98  | PHE  | H    | 8.983      | 0.02        | 1         |
| A     | 73  | LYS  | CD   | 26.27      | 0.3         | 1         |
| A     | 150 | ASP  | HA   | 4.697      | 0.02        | 1         |
| A     | 86  | GLY  | H    | 8.902      | 0.02        | 1         |
| A     | 139 | VAL  | CG2  | 16.492     | 0.3         | 1         |
| A     | 68  | HIS  | CA   | 51.106     | 0.3         | 1         |
| A     | 19  | PRO  | HD2  | 3.653      | 0.02        | 2         |
| A     | 140 | ASP  | H    | 7.794      | 0.02        | 1         |
| A     | 55  | ILE  | HB   | 1.759      | 0.02        | 1         |
| A     | 111 | THR  | CB   | 65.404     | 0.3         | 1         |
| A     | 41  | THR  | H    | 7.459      | 0.02        | 1         |
| A     | 91  | ALA  | H    | 8.581      | 0.02        | 1         |
| A     | 128 | PRO  | CA   | 60.153     | 0.3         | 1         |
| A     | 122 | LEU  | CD1  | 22.163     | 0.3         | 1         |
| A     | 63  | ALA  | CB   | 15.032     | 0.3         | 1         |
| A     | 87  | ILE  | CG2  | 13.428     | 0.3         | 1         |
| A     | 169 | ASN  | HB2  | 2.724      | 0.02        | 2         |
| A     | 37  | TRP  | CB   | 27.639     | 0.3         | 1         |
| A     | 26  | VAL  | CB   | 28.581     | 0.3         | 1         |
| A     | 100 | THR  | H    | 8.338      | 0.02        | 1         |
| A     | 153 | GLY  | HA3  | 3.705      | 0.02        | 2         |
| A     | 149 | ASP  | N    | 117.544    | 0.3         | 1         |
| A     | 10  | ILE  | CB   | 37.489     | 0.3         | 1         |
| A     | 9   | TYR  | HA   | 4.715      | 0.02        | 1         |
| A     | 32  | LYS  | HD3  | 0.827      | 0.02        | 2         |
| A     | 40  | VAL  | CB   | 29.799     | 0.3         | 1         |
| A     | 131 | VAL  | HG12 | 1.121      | 0.02        | 1         |
| A     | 58  | VAL  | HG13 | 0.626      | 0.02        | 1         |
| A     | 76  | ILE  | HD11 | 0.903      | 0.02        | 1         |
| A     | 151 | ILE  | CB   | 35.565     | 0.3         | 1         |
| A     | 52  | MET  | CG   | 32.012     | 0.3         | 1         |
| A     | 43  | LEU  | C    | 173.45     | 0.3         | 1         |
| A     | 157 | LEU  | CD2  | 21.097     | 0.3         | 1         |
| A     | 28  | TYR  | CA   | 58.942     | 0.3         | 1         |
| A     | 79  | HIS  | HB3  | 3.023      | 0.02        | 2         |
| A     | 66  | ASP  | N    | 126.858    | 0.3         | 1         |
| A     | 24  | GLU  | CG   | 33.519     | 0.3         | 1         |
| A     | 46  | SER  | CA   | 53.971     | 0.3         | 1         |
| A     | 40  | VAL  | HG23 | 1.051      | 0.02        | 1         |
| A     | 155 | GLN  | CA   | 55.862     | 0.3         | 1         |
| A     | 105 | GLY  | CA   | 43.136     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 16  | ASN  | CA   | 49.167     | 0.3         | 1         |
| A     | 5   | TRP  | NE1  | 125.655    | 0.3         | 1         |
| A     | 27  | ASP  | HB2  | 2.717      | 0.02        | 2         |
| A     | 142 | ASN  | HB3  | 2.682      | 0.02        | 2         |
| A     | 157 | LEU  | CG   | 24.413     | 0.3         | 1         |
| A     | 24  | GLU  | H    | 9.022      | 0.02        | 1         |
| A     | 36  | VAL  | HG21 | 0.401      | 0.02        | 1         |
| A     | 34  | PHE  | CA   | 61.08      | 0.3         | 1         |
| A     | 13  | ARG  | H    | 8.291      | 0.02        | 1         |
| A     | 78  | ALA  | HB2  | 1.003      | 0.02        | 1         |
| A     | 83  | PRO  | CG   | 24.248     | 0.3         | 1         |
| A     | 128 | PRO  | C    | 175.042    | 0.3         | 1         |
| A     | 133 | PHE  | HA   | 4.854      | 0.02        | 1         |
| A     | 112 | ALA  | HB1  | 0.953      | 0.02        | 1         |
| A     | 98  | PHE  | CB   | 36.429     | 0.3         | 1         |
| A     | 60  | ALA  | C    | 172.015    | 0.3         | 1         |
| A     | 154 | ILE  | HG21 | 1.455      | 0.02        | 1         |
| A     | 120 | LEU  | HB2  | 1.264      | 0.02        | 1         |
| A     | 145 | ARG  | HD2  | 3.032      | 0.02        | 2         |
| A     | 93  | PHE  | HB2  | 2.053      | 0.02        | 1         |
| A     | 62  | GLY  | C    | 173.05     | 0.3         | 1         |
| A     | 101 | THR  | HG23 | 0.434      | 0.02        | 1         |
| A     | 91  | ALA  | CB   | 18.087     | 0.3         | 1         |
| A     | 38  | SER  | CB   | 60.893     | 0.3         | 1         |
| A     | 99  | TRP  | HA   | 4.309      | 0.02        | 1         |
| A     | 101 | THR  | HB   | 4.262      | 0.02        | 1         |
| A     | 48  | ILE  | HD13 | 0.541      | 0.02        | 1         |
| A     | 80  | ALA  | CB   | 16.133     | 0.3         | 1         |
| A     | 132 | MET  | C    | 174.389    | 0.3         | 1         |
| A     | 115 | ALA  | HB3  | 1.06       | 0.02        | 1         |
| A     | 121 | GLY  | HA3  | 3.312      | 0.02        | 2         |
| A     | 61  | ARG  | CG   | 25.953     | 0.3         | 1         |
| A     | 68  | HIS  | N    | 119.701    | 0.3         | 1         |
| A     | 45  | PHE  | HB3  | 2.104      | 0.02        | 2         |
| A     | 78  | ALA  | H    | 7.398      | 0.02        | 1         |
| A     | 40  | VAL  | H    | 7.025      | 0.02        | 1         |
| A     | 66  | ASP  | HB3  | 2.936      | 0.02        | 2         |
| A     | 149 | ASP  | HA   | 4.222      | 0.02        | 1         |
| A     | 58  | VAL  | HG22 | 0.791      | 0.02        | 1         |
| A     | 19  | PRO  | N    | 139.641    | 0.3         | 1         |
| A     | 57  | VAL  | HB   | 2.064      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 23  | ARG  | C    | 175.219    | 0.3         | 1         |
| A     | 74  | GLY  | HA3  | 3.382      | 0.02        | 2         |
| A     | 24  | GLU  | HG2  | 2.201      | 0.02        | 1         |
| A     | 131 | VAL  | HB   | 2.381      | 0.02        | 1         |
| A     | 158 | TYR  | N    | 112.416    | 0.3         | 1         |
| A     | 134 | PRO  | CA   | 60.989     | 0.3         | 1         |
| A     | 9   | TYR  | N    | 119.899    | 0.3         | 1         |
| A     | 107 | ASN  | C    | 173.528    | 0.3         | 1         |
| A     | 41  | THR  | N    | 109.982    | 0.3         | 1         |
| A     | 48  | ILE  | HA   | 4.504      | 0.02        | 1         |
| A     | 87  | ILE  | HG22 | 0.359      | 0.02        | 1         |
| A     | 59  | PHE  | CB   | 38.106     | 0.3         | 1         |
| A     | 150 | ASP  | CA   | 54.95      | 0.3         | 1         |
| A     | 131 | VAL  | C    | 176.244    | 0.3         | 1         |
| A     | 139 | VAL  | CB   | 32.316     | 0.3         | 1         |
| A     | 56  | LEU  | HD23 | 1.012      | 0.02        | 1         |
| A     | 111 | THR  | HA   | 4.021      | 0.02        | 1         |
| A     | 31  | ARG  | CA   | 57.446     | 0.3         | 1         |
| A     | 36  | VAL  | HA   | 3.538      | 0.02        | 1         |
| A     | 151 | ILE  | HD12 | 0.648      | 0.02        | 1         |
| A     | 54  | ASP  | H    | 7.962      | 0.02        | 1         |
| A     | 63  | ALA  | HA   | 4.239      | 0.02        | 1         |
| A     | 157 | LEU  | HD13 | 0.629      | 0.02        | 1         |
| A     | 12  | TYR  | CA   | 52.174     | 0.3         | 1         |
| A     | 106 | THR  | CB   | 65.705     | 0.3         | 1         |
| A     | 154 | ILE  | CD1  | 12.083     | 0.3         | 1         |
| A     | 34  | PHE  | HA   | 3.633      | 0.02        | 1         |
| A     | 107 | ASN  | CB   | 38.909     | 0.3         | 1         |
| A     | 107 | ASN  | HB3  | 3.006      | 0.02        | 2         |
| A     | 14  | ILE  | HB   | 1.614      | 0.02        | 1         |
| A     | 126 | SER  | HA   | 4.657      | 0.02        | 1         |
| A     | 87  | ILE  | CB   | 35.347     | 0.3         | 1         |
| A     | 50  | THR  | CG2  | 17.974     | 0.3         | 1         |
| A     | 47  | LYS  | CA   | 52.434     | 0.3         | 1         |
| A     | 112 | ALA  | C    | 175.911    | 0.3         | 1         |
| A     | 78  | ALA  | CB   | 19.999     | 0.3         | 1         |
| A     | 119 | SER  | HA   | 4.165      | 0.02        | 1         |
| A     | 9   | TYR  | HB2  | 2.748      | 0.02        | 2         |
| A     | 151 | ILE  | HA   | 3.539      | 0.02        | 1         |
| A     | 33  | ALA  | CA   | 52.703     | 0.3         | 1         |
| A     | 139 | VAL  | HG11 | 0.729      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 40  | VAL  | CG2  | 15.979     | 0.3         | 1         |
| A     | 53  | ALA  | HA   | 4.422      | 0.02        | 1         |
| A     | 120 | LEU  | CA   | 52.096     | 0.3         | 1         |
| A     | 47  | LYS  | HE2  | 2.939      | 0.02        | 1         |
| A     | 157 | LEU  | HG   | 1.657      | 0.02        | 1         |
| A     | 150 | ASP  | C    | 175.04     | 0.3         | 1         |
| A     | 18  | THR  | HA   | 4.702      | 0.02        | 1         |
| A     | 97  | GLU  | H    | 9.391      | 0.02        | 1         |
| A     | 109 | PHE  | HB3  | 3.035      | 0.02        | 2         |
| A     | 131 | VAL  | CA   | 61.992     | 0.3         | 1         |
| A     | 11  | THR  | HG21 | 0.968      | 0.02        | 1         |
| A     | 147 | SER  | C    | 172.27     | 0.3         | 1         |
| A     | 148 | ALA  | HB2  | 1.348      | 0.02        | 1         |
| A     | 26  | VAL  | HB   | 2.478      | 0.02        | 1         |
| A     | 39  | ASN  | H    | 8.012      | 0.02        | 1         |
| A     | 160 | ASP  | HA   | 4.555      | 0.02        | 1         |
| A     | 135 | THR  | HB   | 3.959      | 0.02        | 1         |
| A     | 131 | VAL  | HG22 | 0.934      | 0.02        | 1         |
| A     | 19  | PRO  | CA   | 60.248     | 0.3         | 1         |
| A     | 80  | ALA  | HB2  | 1.156      | 0.02        | 1         |
| A     | 36  | VAL  | HG13 | 1.014      | 0.02        | 1         |
| A     | 19  | PRO  | HA   | 4.256      | 0.02        | 1         |
| A     | 145 | ARG  | C    | 171.975    | 0.3         | 1         |
| A     | 43  | LEU  | HD22 | 0.54       | 0.02        | 1         |
| A     | 5   | TRP  | CA   | 52.628     | 0.3         | 1         |
| A     | 149 | ASP  | CB   | 41.001     | 0.3         | 1         |
| A     | 89  | GLY  | C    | 169.466    | 0.3         | 1         |
| A     | 22  | ASN  | H    | 8.82       | 0.02        | 1         |
| A     | 139 | VAL  | C    | 169.317    | 0.3         | 1         |
| A     | 10  | ILE  | N    | 128.394    | 0.3         | 1         |
| A     | 116 | ILE  | N    | 115.625    | 0.3         | 1         |
| A     | 21  | MET  | HG3  | 1.955      | 0.02        | 2         |
| A     | 41  | THR  | CA   | 57.105     | 0.3         | 1         |
| A     | 146 | LEU  | HA   | 3.882      | 0.02        | 1         |
| A     | 141 | ILE  | HG22 | 0.923      | 0.02        | 1         |
| A     | 120 | LEU  | HD21 | 0.732      | 0.02        | 1         |
| A     | 129 | LYS  | HD2  | 2.465      | 0.02        | 2         |
| A     | 53  | ALA  | CA   | 46.873     | 0.3         | 1         |
| A     | 62  | GLY  | H    | 9.407      | 0.02        | 1         |
| A     | 41  | THR  | HG22 | 1.379      | 0.02        | 1         |
| A     | 110 | LEU  | HG   | 0.92       | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 76  | ILE  | HG21 | 1.164      | 0.02        | 1         |
| A     | 38  | SER  | HA   | 4.199      | 0.02        | 1         |
| A     | 10  | ILE  | HD12 | 0.014      | 0.02        | 1         |
| A     | 128 | PRO  | HA   | 2.464      | 0.02        | 1         |
| A     | 108 | LEU  | HB2  | 1.657      | 0.02        | 2         |
| A     | 156 | SER  | C    | 172.161    | 0.3         | 1         |
| A     | 51  | GLY  | C    | 170.557    | 0.3         | 1         |
| A     | 110 | LEU  | CD1  | 20.856     | 0.3         | 1         |
| A     | 9   | TYR  | CB   | 35.46      | 0.3         | 1         |
| A     | 26  | VAL  | CG2  | 18.584     | 0.3         | 1         |
| A     | 120 | LEU  | HD23 | 0.732      | 0.02        | 1         |
| A     | 58  | VAL  | HG12 | 0.626      | 0.02        | 1         |
| A     | 114 | HIS  | CB   | 26.379     | 0.3         | 1         |
| A     | 64  | HIS  | C    | 173.48     | 0.3         | 1         |
| A     | 74  | GLY  | CA   | 40.107     | 0.3         | 1         |
| A     | 59  | PHE  | HB3  | 2.857      | 0.02        | 2         |
| A     | 139 | VAL  | HG21 | 0.675      | 0.02        | 1         |
| A     | 76  | ILE  | CG1  | 25.325     | 0.3         | 1         |
| A     | 98  | PHE  | N    | 119.21     | 0.3         | 1         |
| A     | 77  | LEU  | HD11 | -0.036     | 0.02        | 1         |
| A     | 30  | ILE  | HG23 | 0.64       | 0.02        | 1         |
| A     | 109 | PHE  | CB   | 34.896     | 0.3         | 1         |
| A     | 110 | LEU  | N    | 117.948    | 0.3         | 1         |
| A     | 96  | ASP  | C    | 176.687    | 0.3         | 1         |
| A     | 73  | LYS  | HB2  | 1.502      | 0.02        | 1         |
| A     | 100 | THR  | HB   | 4.432      | 0.02        | 1         |
| A     | 133 | PHE  | CB   | 37.639     | 0.3         | 1         |
| A     | 62  | GLY  | HA2  | 3.851      | 0.02        | 2         |
| A     | 91  | ALA  | N    | 119.865    | 0.3         | 1         |
| A     | 37  | TRP  | HB2  | 3.059      | 0.02        | 2         |
| A     | 129 | LYS  | HG2  | 1.384      | 0.02        | 2         |
| A     | 113 | VAL  | HB   | 1.602      | 0.02        | 1         |
| A     | 26  | VAL  | HG22 | 0.784      | 0.02        | 1         |
| A     | 152 | ARG  | N    | 119.13     | 0.3         | 1         |
| A     | 66  | ASP  | CA   | 59.227     | 0.3         | 1         |
| A     | 47  | LYS  | HB2  | 1.355      | 0.02        | 2         |
| A     | 125 | SER  | N    | 113.754    | 0.3         | 1         |
| A     | 146 | LEU  | HD13 | 1.166      | 0.02        | 1         |
| A     | 20  | ASP  | HA   | 3.987      | 0.02        | 1         |
| A     | 149 | ASP  | H    | 8.18       | 0.02        | 1         |
| A     | 53  | ALA  | C    | 173.643    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 139 | VAL  | CG1  | 18.263     | 0.3         | 1         |
| A     | 116 | ILE  | HG12 | 0.943      | 0.02        | 2         |
| A     | 132 | MET  | HB2  | 2.565      | 0.02        | 2         |
| A     | 55  | ILE  | HA   | 4.072      | 0.02        | 1         |
| A     | 70  | PHE  | C    | 173.477    | 0.3         | 1         |
| A     | 22  | ASN  | ND2  | 113.938    | 0.3         | 1         |
| A     | 76  | ILE  | C    | 174.175    | 0.3         | 1         |
| A     | 138 | TYR  | CA   | 58.346     | 0.3         | 1         |
| A     | 34  | PHE  | HB2  | 2.477      | 0.02        | 1         |
| A     | 110 | LEU  | C    | 176.089    | 0.3         | 1         |
| A     | 146 | LEU  | N    | 121.116    | 0.3         | 1         |
| A     | 10  | ILE  | CA   | 56.317     | 0.3         | 1         |
| A     | 111 | THR  | C    | 173.916    | 0.3         | 1         |
| A     | 116 | ILE  | CA   | 60.522     | 0.3         | 1         |
| A     | 129 | LYS  | HE2  | 2.882      | 0.02        | 1         |
| A     | 113 | VAL  | N    | 118.495    | 0.3         | 1         |
| A     | 59  | PHE  | N    | 125.471    | 0.3         | 1         |
| A     | 90  | ASP  | CB   | 36.867     | 0.3         | 1         |
| A     | 53  | ALA  | N    | 126.941    | 0.3         | 1         |
| A     | 85  | SER  | HA   | 4.349      | 0.02        | 1         |
| A     | 46  | SER  | CB   | 63.031     | 0.3         | 1         |
| A     | 22  | ASN  | N    | 118.643    | 0.3         | 1         |
| A     | 160 | ASP  | CB   | 36.504     | 0.3         | 1         |
| A     | 142 | ASN  | ND2  | 115.129    | 0.3         | 1         |

## 7.2.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 344      | $2.59 \pm 0.09$                 | Should be applied          |
| $^{13}\text{C}_\beta$  | 313      | $2.79 \pm 0.18$                 | Should be applied          |
| $^{13}\text{C}'$       | 338      | $3.09 \pm 0.07$                 | Should be applied          |
| $^{15}\text{N}$        | 342      | $0.22 \pm 0.41$                 | None needed ( $< 0.5$ ppm) |

## 7.2.3 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 74%, i.e. 1874 atoms were assigned a chemical shift out of a possible 2546. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.



|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 909/926 (98%)   | 362/368 (98%)  | 371/380 (98%)   | 176/178 (99%)   |
| Sidechain | 955/1250 (76%)  | 569/746 (76%)  | 370/438 (84%)   | 16/66 (24%)     |
| Aromatic  | 10/370 (3%)     | 5/196 (3%)     | 0/167 (0%)      | 5/7 (71%)       |
| Overall   | 1874/2546 (74%) | 936/1310 (71%) | 741/985 (75%)   | 197/251 (78%)   |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1893 atoms were assigned a chemical shift out of a possible 2590. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 917/944 (97%)   | 365/375 (97%)  | 375/388 (97%)   | 177/181 (98%)   |
| Sidechain | 966/1276 (76%)  | 576/762 (76%)  | 374/448 (83%)   | 16/66 (24%)     |
| Aromatic  | 10/370 (3%)     | 5/196 (3%)     | 0/167 (0%)      | 5/7 (71%)       |
| Overall   | 1893/2590 (73%) | 946/1333 (71%) | 749/1003 (75%)  | 198/254 (78%)   |

#### 7.2.4 Statistically unusual chemical shifts ⓘ

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

| Mol | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|-----|-------|-----|------|------|------------|---------------------|---------|
| 1   | A     | 392 | THR  | HG22 | -1.19      | 2.29 – -0.01        | -10.1   |
| 1   | A     | 392 | THR  | HG23 | -1.19      | 2.29 – -0.01        | -10.1   |
| 1   | A     | 392 | THR  | HG21 | -1.19      | 2.29 – -0.01        | -10.1   |
| 1   | A     | 450 | GLU  | HG3  | 0.81       | 3.31 – 1.21         | -6.9    |
| 1   | A     | 298 | ILE  | HG21 | -0.94      | 2.13 – -0.57        | -6.4    |
| 1   | A     | 298 | ILE  | HG23 | -0.94      | 2.13 – -0.57        | -6.4    |
| 1   | A     | 298 | ILE  | HG22 | -0.94      | 2.13 – -0.57        | -6.4    |
| 1   | A     | 410 | MET  | CG   | 24.07      | 38.33 – 25.73       | -6.3    |
| 1   | A     | 134 | PRO  | CB   | 24.69      | 37.79 – 25.89       | -6.0    |
| 1   | A     | 128 | PRO  | HA   | 2.46       | 6.05 – 2.75         | -5.9    |
| 1   | A     | 425 | ILE  | HG21 | -0.79      | 2.13 – -0.57        | -5.8    |
| 1   | A     | 425 | ILE  | HG23 | -0.79      | 2.13 – -0.57        | -5.8    |
| 1   | A     | 425 | ILE  | HG22 | -0.79      | 2.13 – -0.57        | -5.8    |
| 1   | A     | 106 | THR  | HB   | 2.35       | 5.82 – 2.52         | -5.5    |
| 1   | A     | 352 | TYR  | HB3  | 0.91       | 4.75 – 0.95         | -5.1    |
| 1   | A     | 448 | GLN  | HG3  | 0.83       | 3.75 – 0.85         | -5.1    |
| 1   | A     | 380 | ILE  | HD13 | -0.79      | 2.13 – -0.77        | -5.1    |
| 1   | A     | 380 | ILE  | HD12 | -0.79      | 2.13 – -0.77        | -5.1    |
| 1   | A     | 380 | ILE  | HD11 | -0.79      | 2.13 – -0.77        | -5.1    |

### 7.2.5 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.

Random coil index (RCI) for chain A:

