



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:15 PM BST

PDB ID : 1PZQ  
Title : Structure of fused docking domains from the erythromycin polyketide synthase (DEBS), a model for the interaction between DEBS 2 and DEBS 3: The A domain  
Authors : Broadhurst, R.W.; Nietlispach, D.; Wheatcroft, M.P.; Leadlay, P.F.; Weissman, K.J.  
Deposited on : 2003-07-14

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  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

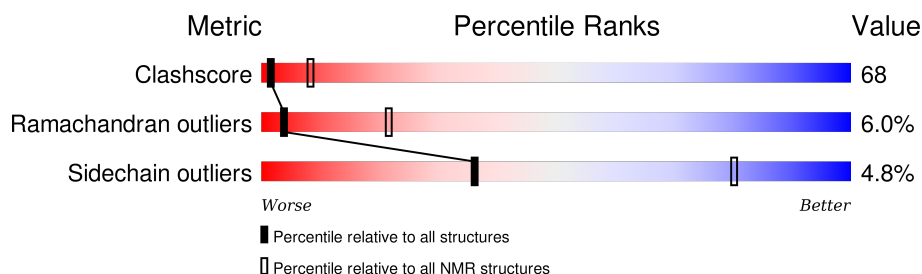
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

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            | 114402                      | 11133                     |
| Ramachandran outliers | 111179                      | 9975                      |
| Sidechain outliers    | 111093                      | 9958                      |

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     | 60     |                  |
| 1   | B     | 60     |                  |

## 2 Ensemble composition and analysis ⓘ

This entry contains 8 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:7-A:49, B:7-B:49 (86) | 0.14              | 7            |

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1758 atoms, of which 856 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Erythronolide synthase.

| Mol | Chain | Residues | Atoms |     |     |    |     | Trace |
|-----|-------|----------|-------|-----|-----|----|-----|-------|
| 1   | A     | 60       | Total | C   | H   | N  | O   | 0     |
|     |       |          | 879   | 267 | 428 | 84 | 100 |       |
| 1   | B     | 60       | Total | C   | H   | N  | O   | 0     |
|     |       |          | 879   | 267 | 428 | 84 | 100 |       |

There are 4 discrepancies between the modelled and reference sequences:

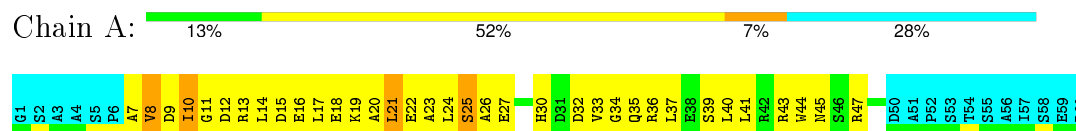
| Chain | Residue | Modelled | Actual | Comment          | Reference  |
|-------|---------|----------|--------|------------------|------------|
| A     | 1       | GLY      | -      | CLONING ARTIFACT | UNP Q03132 |
| A     | 2       | SER      | -      | CLONING ARTIFACT | UNP Q03132 |
| B     | 1       | GLY      | -      | CLONING ARTIFACT | UNP Q03132 |
| B     | 2       | SER      | -      | CLONING ARTIFACT | UNP Q03132 |

## 4 Residue-property plots

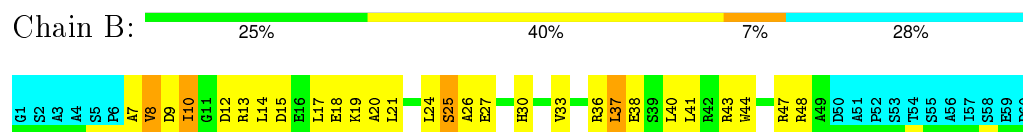
### 4.1 Average score per residue in the NMR ensemble

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: Erythronolide synthase



- Molecule 1: Erythronolide synthase

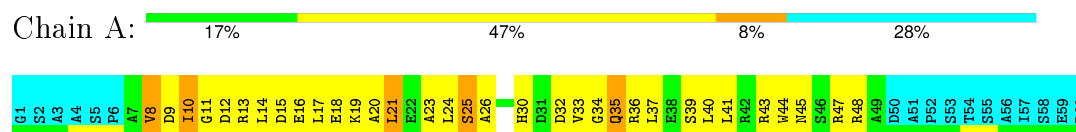


### 4.2 Scores per residue for each member of the ensemble

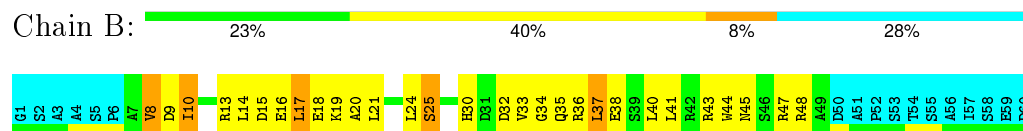
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Erythronolide synthase

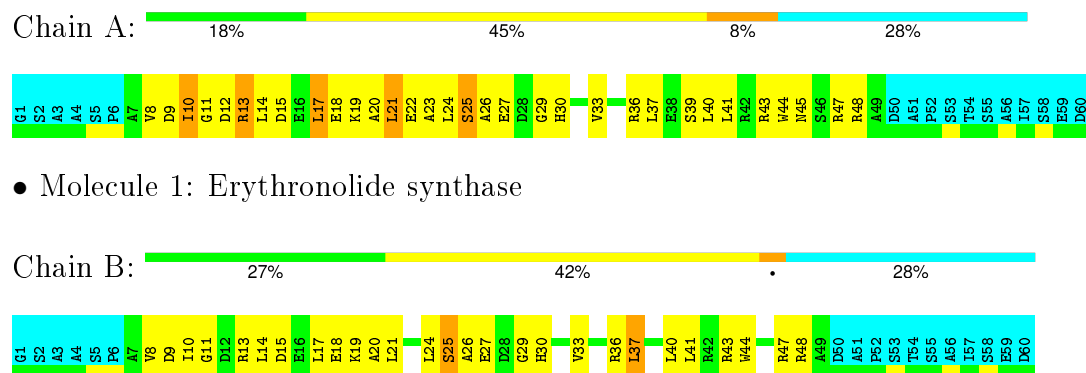


- Molecule 1: Erythronolide synthase



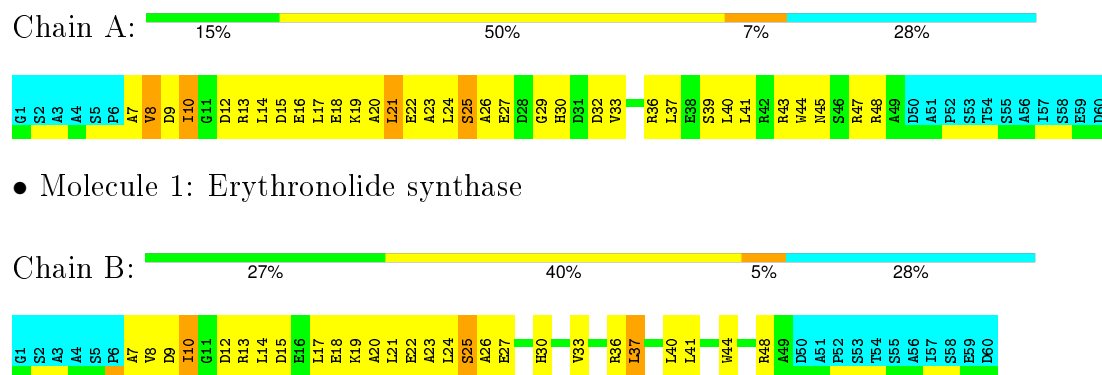
### 4.2.2 Score per residue for model 2

- Molecule 1: Erythronolide synthase



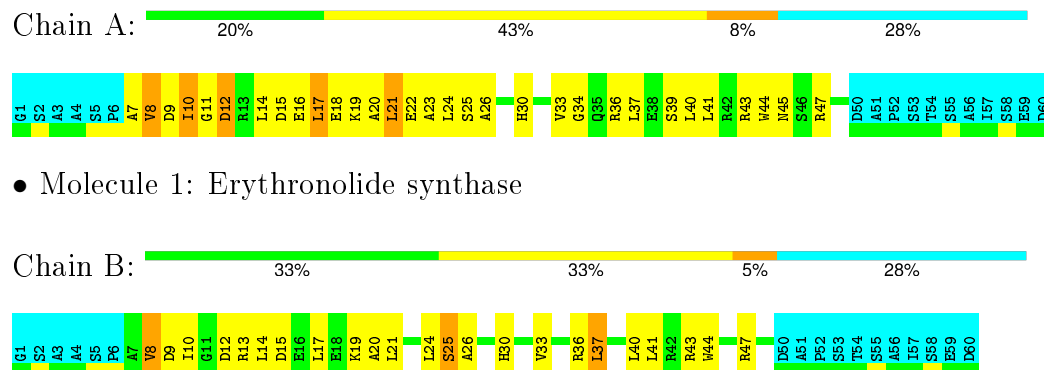
### 4.2.3 Score per residue for model 3

- Molecule 1: Erythronolide synthase



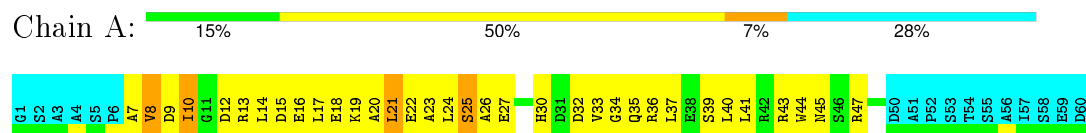
### 4.2.4 Score per residue for model 4

- Molecule 1: Erythronolide synthase

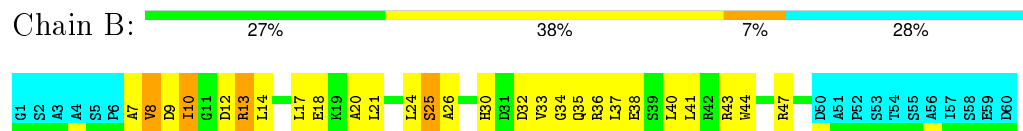


### 4.2.5 Score per residue for model 5

- Molecule 1: Erythronolide synthase

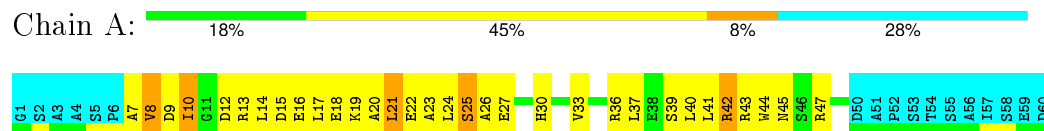


- Molecule 1: Erythronolide synthase

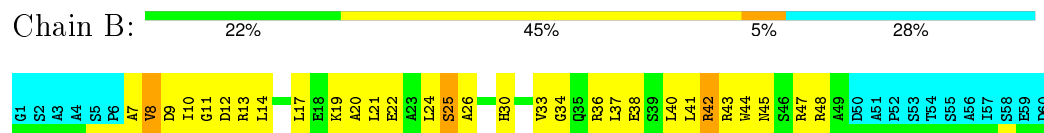


### 4.2.6 Score per residue for model 6

- Molecule 1: Erythronolide synthase

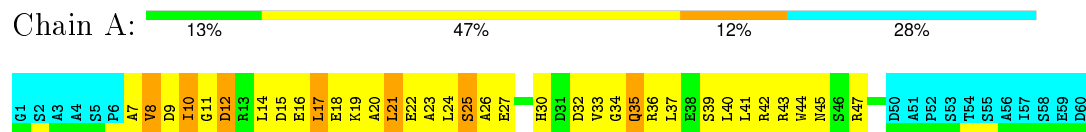


- Molecule 1: Erythronolide synthase

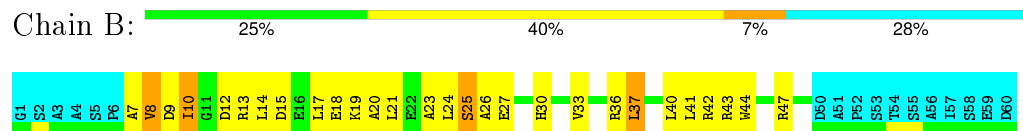


### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Erythronolide synthase

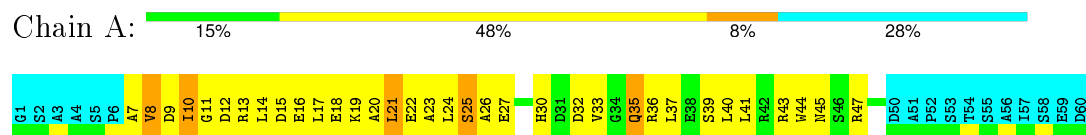


- Molecule 1: Erythronolide synthase

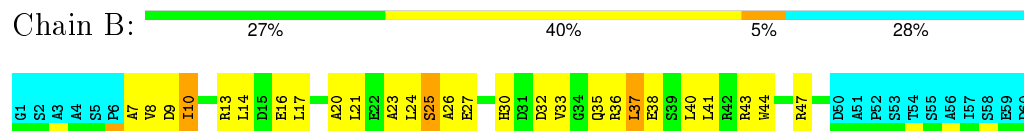


## 4.2.8 Score per residue for model 8

### • Molecule 1: Erythronolide synthase



### • Molecule 1: Erythronolide synthase





## 5 Refinement protocol and experimental data overview

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

Of the 40 calculated structures, 8 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CNS           | structure solution | 1.0     |
| CNS           | refinement         | 1.0     |

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 5885 |
| Number of chemical shift lists               | 1               |
| Total number of shifts                       | 2358            |
| Number of shifts mapped to atoms             | 1136            |
| Number of unparsed shifts                    | 0               |
| Number of shifts with mapping errors         | 1222            |
| Number of shifts with mapping warnings       | 0               |
| Assignment completeness (well-defined parts) | 80%             |

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1   | A     | 342   | 332      | 331      | 75±5    |
| 1   | B     | 342   | 332      | 331      | 59±5    |
| All | All   | 5472  | 5312     | 5296     | 735     |

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 68.

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

| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:21:LEU:HD11 | 1:A:33:VAL:HG11 | 0.93     | 1.40        | 5      | 8     |
| 1:A:18:GLU:HB2  | 1:B:40:LEU:HD22 | 0.91     | 1.43        | 1      | 2     |
| 1:A:17:LEU:HD21 | 1:B:14:LEU:HD13 | 0.85     | 1.46        | 2      | 1     |
| 1:A:24:LEU:HD13 | 1:B:10:ILE:HD13 | 0.84     | 1.49        | 3      | 5     |
| 1:A:10:ILE:HG21 | 1:B:33:VAL:HG22 | 0.84     | 1.47        | 1      | 8     |
| 1:A:41:LEU:HD22 | 1:A:45:ASN:ND2  | 0.79     | 1.92        | 1      | 8     |
| 1:A:40:LEU:HD13 | 1:B:17:LEU:HD23 | 0.79     | 1.52        | 2      | 2     |
| 1:B:9:ASP:O     | 1:B:10:ILE:HG22 | 0.78     | 1.79        | 8      | 8     |
| 1:B:10:ILE:O    | 1:B:14:LEU:HD23 | 0.75     | 1.81        | 4      | 2     |
| 1:A:14:LEU:HG   | 1:B:17:LEU:HD11 | 0.75     | 1.57        | 8      | 7     |
| 1:A:15:ASP:O    | 1:A:19:LYS:HG3  | 0.72     | 1.85        | 3      | 1     |
| 1:A:44:TRP:CZ2  | 1:B:33:VAL:HB   | 0.71     | 2.20        | 1      | 8     |
| 1:A:13:ARG:NH1  | 1:B:20:ALA:HB2  | 0.71     | 2.00        | 8      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:47:ARG:HD3  | 1:B:25:SER:HB2  | 0.71     | 1.61        | 3      | 7     |
| 1:A:8:VAL:HG13  | 1:A:12:ASP:HB3  | 0.71     | 1.61        | 6      | 3     |
| 1:A:21:LEU:CD1  | 1:A:33:VAL:HG11 | 0.70     | 2.17        | 5      | 8     |
| 1:A:17:LEU:HA   | 1:B:13:ARG:HE   | 0.70     | 1.46        | 2      | 1     |
| 1:A:33:VAL:HG22 | 1:B:10:ILE:HG21 | 0.69     | 1.62        | 5      | 8     |
| 1:B:10:ILE:HA   | 1:B:13:ARG:NH1  | 0.69     | 2.02        | 2      | 1     |
| 1:A:13:ARG:HH11 | 1:B:20:ALA:HB2  | 0.69     | 1.47        | 8      | 1     |
| 1:A:40:LEU:HD11 | 1:B:14:LEU:HD12 | 0.69     | 1.64        | 2      | 1     |
| 1:A:37:LEU:HA   | 1:A:40:LEU:HD12 | 0.69     | 1.64        | 2      | 2     |
| 1:A:14:LEU:HD23 | 1:B:40:LEU:HD11 | 0.68     | 1.63        | 2      | 5     |
| 1:A:24:LEU:HD23 | 1:B:10:ILE:HD13 | 0.68     | 1.65        | 4      | 3     |
| 1:A:33:VAL:HG13 | 1:B:14:LEU:HD11 | 0.68     | 1.65        | 8      | 1     |
| 1:A:17:LEU:HD23 | 1:B:40:LEU:HD13 | 0.68     | 1.64        | 8      | 1     |
| 1:A:17:LEU:HD11 | 1:B:14:LEU:HG   | 0.67     | 1.65        | 8      | 3     |
| 1:A:8:VAL:HG13  | 1:A:12:ASP:HB2  | 0.66     | 1.66        | 7      | 3     |
| 1:A:10:ILE:HD12 | 1:A:13:ARG:HG3  | 0.66     | 1.67        | 3      | 3     |
| 1:A:10:ILE:O    | 1:A:13:ARG:NH1  | 0.65     | 2.29        | 2      | 1     |
| 1:A:36:ARG:O    | 1:A:40:LEU:HG   | 0.65     | 1.91        | 1      | 8     |
| 1:A:17:LEU:HD21 | 1:B:14:LEU:HD22 | 0.64     | 1.67        | 4      | 1     |
| 1:A:17:LEU:HD13 | 1:B:13:ARG:HB2  | 0.64     | 1.69        | 1      | 1     |
| 1:A:41:LEU:HD22 | 1:A:45:ASN:HD21 | 0.63     | 1.52        | 1      | 8     |
| 1:A:13:ARG:NH2  | 1:B:17:LEU:HG   | 0.63     | 2.08        | 2      | 1     |
| 1:A:21:LEU:HD12 | 1:B:44:TRP:CZ3  | 0.62     | 2.29        | 4      | 8     |
| 1:B:36:ARG:O    | 1:B:40:LEU:HG   | 0.62     | 1.94        | 1      | 7     |
| 1:A:32:ASP:O    | 1:A:35:GLN:HG2  | 0.62     | 1.94        | 5      | 3     |
| 1:A:36:ARG:CB   | 1:B:14:LEU:HG   | 0.62     | 2.25        | 2      | 2     |
| 1:A:36:ARG:HB2  | 1:B:14:LEU:HD13 | 0.61     | 1.72        | 7      | 5     |
| 1:A:37:LEU:HG   | 1:B:14:LEU:HD21 | 0.61     | 1.72        | 3      | 4     |
| 1:A:20:ALA:HB2  | 1:B:13:ARG:HH11 | 0.61     | 1.55        | 8      | 1     |
| 1:A:41:LEU:HG   | 1:B:37:LEU:HG   | 0.61     | 1.71        | 6      | 2     |
| 1:B:21:LEU:O    | 1:B:25:SER:N    | 0.59     | 2.35        | 2      | 8     |
| 1:A:39:SER:O    | 1:A:43:ARG:HG2  | 0.59     | 1.97        | 3      | 8     |
| 1:A:40:LEU:CD2  | 1:B:18:GLU:HB2  | 0.59     | 2.27        | 1      | 5     |
| 1:A:8:VAL:O     | 1:A:12:ASP:HB2  | 0.59     | 1.98        | 2      | 3     |
| 1:B:8:VAL:HG13  | 1:B:12:ASP:HB3  | 0.59     | 1.73        | 3      | 3     |
| 1:A:13:ARG:HB2  | 1:A:13:ARG:NH1  | 0.58     | 2.13        | 2      | 1     |
| 1:A:13:ARG:HB2  | 1:A:13:ARG:CZ   | 0.58     | 2.27        | 2      | 1     |
| 1:B:24:LEU:HD22 | 1:B:24:LEU:N    | 0.57     | 2.14        | 5      | 2     |
| 1:A:40:LEU:HB3  | 1:B:37:LEU:HD21 | 0.57     | 1.75        | 6      | 2     |
| 1:B:32:ASP:O    | 1:B:35:GLN:HG2  | 0.57     | 1.98        | 1      | 3     |
| 1:A:17:LEU:HD22 | 1:B:13:ARG:NH2  | 0.57     | 2.14        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:B:24:LEU:O    | 1:B:26:ALA:N    | 0.57     | 2.37        | 6      | 7     |
| 1:A:17:LEU:HD22 | 1:B:13:ARG:CZ   | 0.57     | 2.29        | 2      | 1     |
| 1:A:17:LEU:CD2  | 1:B:17:LEU:HD12 | 0.57     | 2.29        | 1      | 1     |
| 1:A:42:ARG:HD3  | 1:A:42:ARG:O    | 0.57     | 1.99        | 7      | 1     |
| 1:A:21:LEU:HD13 | 1:B:10:ILE:HD11 | 0.56     | 1.75        | 2      | 8     |
| 1:B:24:LEU:N    | 1:B:24:LEU:HD22 | 0.56     | 2.15        | 6      | 1     |
| 1:B:21:LEU:HD22 | 1:B:33:VAL:HG11 | 0.56     | 1.76        | 7      | 6     |
| 1:A:24:LEU:CD2  | 1:B:10:ILE:HD13 | 0.56     | 2.31        | 4      | 3     |
| 1:B:8:VAL:HG13  | 1:B:12:ASP:HB2  | 0.56     | 1.76        | 7      | 1     |
| 1:A:41:LEU:HA   | 1:A:44:TRP:HB3  | 0.56     | 1.78        | 4      | 8     |
| 1:B:10:ILE:HA   | 1:B:13:ARG:HH12 | 0.56     | 1.59        | 2      | 1     |
| 1:A:33:VAL:HG22 | 1:B:10:ILE:CG2  | 0.56     | 2.30        | 5      | 7     |
| 1:A:40:LEU:HB3  | 1:B:37:LEU:HD11 | 0.56     | 1.76        | 7      | 6     |
| 1:A:41:LEU:O    | 1:A:44:TRP:N    | 0.55     | 2.40        | 1      | 8     |
| 1:A:29:GLY:HA2  | 1:B:48:ARG:HH22 | 0.55     | 1.61        | 3      | 2     |
| 1:A:24:LEU:HD22 | 1:B:10:ILE:HB   | 0.55     | 1.78        | 6      | 4     |
| 1:A:15:ASP:O    | 1:A:19:LYS:HG2  | 0.55     | 2.02        | 2      | 7     |
| 1:A:17:LEU:HD21 | 1:B:14:LEU:HD23 | 0.55     | 1.79        | 8      | 2     |
| 1:A:9:ASP:O     | 1:A:10:ILE:HG22 | 0.54     | 2.02        | 3      | 5     |
| 1:A:24:LEU:O    | 1:A:26:ALA:N    | 0.54     | 2.40        | 1      | 8     |
| 1:A:13:ARG:HE   | 1:B:17:LEU:HA   | 0.54     | 1.61        | 2      | 1     |
| 1:A:17:LEU:HD13 | 1:B:13:ARG:NH2  | 0.54     | 2.18        | 2      | 1     |
| 1:B:24:LEU:HB3  | 1:B:30:HIS:CD2  | 0.54     | 2.38        | 7      | 5     |
| 1:A:9:ASP:O     | 1:A:11:GLY:N    | 0.54     | 2.39        | 2      | 5     |
| 1:B:8:VAL:HG13  | 1:B:8:VAL:O     | 0.54     | 2.02        | 5      | 6     |
| 1:A:37:LEU:HB3  | 1:B:41:LEU:HD13 | 0.54     | 1.79        | 1      | 2     |
| 1:A:17:LEU:HD12 | 1:B:17:LEU:HD23 | 0.54     | 1.79        | 3      | 1     |
| 1:A:14:LEU:HG   | 1:B:17:LEU:HD21 | 0.54     | 1.79        | 1      | 1     |
| 1:A:10:ILE:CG2  | 1:A:11:GLY:N    | 0.54     | 2.71        | 2      | 5     |
| 1:A:13:ARG:CB   | 1:B:17:LEU:HD13 | 0.54     | 2.33        | 3      | 1     |
| 1:A:37:LEU:CB   | 1:B:41:LEU:HD13 | 0.53     | 2.34        | 3      | 2     |
| 1:A:36:ARG:HB3  | 1:B:14:LEU:HG   | 0.53     | 1.80        | 2      | 1     |
| 1:A:30:HIS:HB3  | 1:A:33:VAL:HG23 | 0.53     | 1.81        | 8      | 8     |
| 1:A:11:GLY:HA3  | 1:B:36:ARG:NH1  | 0.53     | 2.19        | 2      | 1     |
| 1:A:14:LEU:HG   | 1:B:17:LEU:CD1  | 0.53     | 2.31        | 8      | 3     |
| 1:A:17:LEU:HD22 | 1:B:13:ARG:HB3  | 0.53     | 1.80        | 4      | 1     |
| 1:B:11:GLY:HA2  | 1:B:14:LEU:HD23 | 0.53     | 1.81        | 2      | 1     |
| 1:A:12:ASP:O    | 1:A:16:GLU:HG3  | 0.52     | 2.04        | 5      | 7     |
| 1:B:15:ASP:O    | 1:B:19:LYS:HD3  | 0.52     | 2.04        | 2      | 1     |
| 1:A:17:LEU:HD11 | 1:B:14:LEU:CD2  | 0.52     | 2.34        | 6      | 1     |
| 1:B:8:VAL:O     | 1:B:8:VAL:HG13  | 0.52     | 2.04        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:17:LEU:HD13 | 1:B:13:ARG:HH21 | 0.52     | 1.63        | 2      | 1     |
| 1:A:13:ARG:HB2  | 1:B:17:LEU:HD13 | 0.52     | 1.80        | 3      | 1     |
| 1:A:23:ALA:O    | 1:A:27:GLU:HG3  | 0.52     | 2.05        | 6      | 5     |
| 1:A:17:LEU:HD22 | 1:B:13:ARG:CB   | 0.52     | 2.34        | 4      | 2     |
| 1:A:17:LEU:CD1  | 1:B:17:LEU:HD23 | 0.52     | 2.35        | 3      | 1     |
| 1:B:10:ILE:O    | 1:B:14:LEU:HD22 | 0.52     | 2.03        | 2      | 1     |
| 1:A:17:LEU:CD1  | 1:B:14:LEU:HD22 | 0.52     | 2.35        | 6      | 1     |
| 1:B:43:ARG:HB3  | 1:B:47:ARG:NH1  | 0.51     | 2.20        | 6      | 2     |
| 1:A:24:LEU:N    | 1:A:24:LEU:HD22 | 0.51     | 2.21        | 8      | 3     |
| 1:A:13:ARG:HB3  | 1:B:17:LEU:HG   | 0.51     | 1.81        | 1      | 1     |
| 1:A:37:LEU:HB3  | 1:B:41:LEU:CG   | 0.51     | 2.35        | 2      | 6     |
| 1:A:10:ILE:HD11 | 1:B:21:LEU:HD23 | 0.51     | 1.81        | 7      | 5     |
| 1:A:21:LEU:CD1  | 1:B:44:TRP:CZ3  | 0.51     | 2.94        | 7      | 8     |
| 1:A:10:ILE:HG13 | 1:A:13:ARG:NH1  | 0.51     | 2.21        | 2      | 1     |
| 1:A:18:GLU:O    | 1:A:22:GLU:HG3  | 0.51     | 2.05        | 2      | 7     |
| 1:A:37:LEU:HG   | 1:B:14:LEU:HD11 | 0.51     | 1.82        | 6      | 2     |
| 1:A:42:ARG:O    | 1:A:42:ARG:HD3  | 0.51     | 2.05        | 6      | 1     |
| 1:B:43:ARG:HB3  | 1:B:47:ARG:HH12 | 0.51     | 1.64        | 6      | 1     |
| 1:A:40:LEU:HD11 | 1:B:14:LEU:HD13 | 0.51     | 1.81        | 4      | 1     |
| 1:A:16:GLU:HB3  | 1:B:13:ARG:NH1  | 0.50     | 2.21        | 5      | 4     |
| 1:A:41:LEU:O    | 1:A:45:ASN:N    | 0.50     | 2.44        | 6      | 7     |
| 1:B:33:VAL:O    | 1:B:37:LEU:HB2  | 0.50     | 2.05        | 8      | 3     |
| 1:A:41:LEU:HG   | 1:B:37:LEU:HD22 | 0.50     | 1.83        | 1      | 5     |
| 1:B:24:LEU:HG   | 1:B:30:HIS:CD2  | 0.50     | 2.41        | 2      | 2     |
| 1:A:35:GLN:HG2  | 1:A:36:ARG:NH1  | 0.50     | 2.22        | 7      | 1     |
| 1:A:18:GLU:HB2  | 1:B:40:LEU:CD2  | 0.50     | 2.34        | 3      | 6     |
| 1:A:17:LEU:HD11 | 1:B:14:LEU:HD22 | 0.50     | 1.82        | 6      | 1     |
| 1:B:41:LEU:HA   | 1:B:44:TRP:HB3  | 0.50     | 1.83        | 8      | 6     |
| 1:B:45:ASN:HA   | 1:B:48:ARG:HD3  | 0.50     | 1.83        | 1      | 2     |
| 1:A:8:VAL:O     | 1:A:12:ASP:HB3  | 0.50     | 2.07        | 1      | 1     |
| 1:A:20:ALA:HA   | 1:B:7:ALA:H     | 0.50     | 1.67        | 3      | 1     |
| 1:A:10:ILE:HD11 | 1:B:21:LEU:HD12 | 0.49     | 1.84        | 1      | 1     |
| 1:A:45:ASN:HA   | 1:A:48:ARG:HD3  | 0.49     | 1.82        | 1      | 1     |
| 1:B:36:ARG:O    | 1:B:40:LEU:HD13 | 0.49     | 2.08        | 5      | 1     |
| 1:A:30:HIS:HB3  | 1:A:33:VAL:CG2  | 0.49     | 2.37        | 4      | 8     |
| 1:A:24:LEU:HD12 | 1:A:30:HIS:NE2  | 0.49     | 2.22        | 4      | 1     |
| 1:A:20:ALA:O    | 1:A:23:ALA:HB3  | 0.49     | 2.07        | 2      | 8     |
| 1:A:20:ALA:HB3  | 1:B:13:ARG:CZ   | 0.49     | 2.38        | 2      | 1     |
| 1:A:40:LEU:HD21 | 1:B:18:GLU:HB2  | 0.49     | 1.83        | 5      | 2     |
| 1:B:8:VAL:O     | 1:B:9:ASP:HB3   | 0.49     | 2.08        | 5      | 2     |
| 1:A:20:ALA:CB   | 1:B:13:ARG:CZ   | 0.48     | 2.90        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:37:LEU:HB3  | 1:B:41:LEU:HG   | 0.48     | 1.86        | 2      | 6     |
| 1:A:44:TRP:CE3  | 1:B:21:LEU:HD23 | 0.48     | 2.43        | 1      | 1     |
| 1:B:20:ALA:O    | 1:B:24:LEU:HD12 | 0.48     | 2.08        | 8      | 1     |
| 1:B:10:ILE:CG2  | 1:B:11:GLY:N    | 0.48     | 2.76        | 2      | 2     |
| 1:A:11:GLY:O    | 1:A:15:ASP:HB2  | 0.48     | 2.08        | 8      | 4     |
| 1:A:10:ILE:O    | 1:A:14:LEU:HD12 | 0.48     | 2.08        | 8      | 2     |
| 1:A:9:ASP:HB2   | 1:A:12:ASP:OD1  | 0.48     | 2.09        | 7      | 2     |
| 1:A:26:ALA:HB2  | 1:B:48:ARG:HA   | 0.47     | 1.86        | 2      | 1     |
| 1:A:36:ARG:HB2  | 1:B:14:LEU:HG   | 0.47     | 1.86        | 6      | 2     |
| 1:A:32:ASP:O    | 1:A:36:ARG:HG2  | 0.47     | 2.09        | 1      | 5     |
| 1:B:8:VAL:O     | 1:B:9:ASP:HB2   | 0.47     | 2.09        | 7      | 5     |
| 1:A:7:ALA:CB    | 1:B:24:LEU:HD11 | 0.47     | 2.39        | 8      | 2     |
| 1:A:41:LEU:HD11 | 1:B:38:GLU:CA   | 0.47     | 2.40        | 1      | 4     |
| 1:A:41:LEU:HG   | 1:B:37:LEU:HB3  | 0.47     | 1.87        | 3      | 1     |
| 1:B:8:VAL:CG1   | 1:B:13:ARG:HG3  | 0.47     | 2.39        | 8      | 2     |
| 1:A:21:LEU:HD21 | 1:A:33:VAL:CG1  | 0.47     | 2.39        | 2      | 2     |
| 1:A:40:LEU:HB2  | 1:B:37:LEU:HD21 | 0.47     | 1.87        | 4      | 3     |
| 1:A:36:ARG:CB   | 1:B:14:LEU:HD13 | 0.47     | 2.40        | 3      | 3     |
| 1:B:10:ILE:O    | 1:B:13:ARG:NH1  | 0.47     | 2.48        | 2      | 1     |
| 1:A:24:LEU:HD12 | 1:A:30:HIS:CD2  | 0.47     | 2.45        | 4      | 2     |
| 1:A:44:TRP:CE2  | 1:B:33:VAL:HB   | 0.46     | 2.45        | 5      | 8     |
| 1:A:7:ALA:CB    | 1:B:24:LEU:HD21 | 0.46     | 2.40        | 5      | 2     |
| 1:A:23:ALA:CB   | 1:B:7:ALA:HB2   | 0.46     | 2.39        | 6      | 3     |
| 1:B:13:ARG:HB2  | 1:B:13:ARG:CZ   | 0.46     | 2.39        | 2      | 1     |
| 1:A:37:LEU:O    | 1:A:40:LEU:HB2  | 0.46     | 2.10        | 6      | 5     |
| 1:A:17:LEU:HD11 | 1:B:14:LEU:HD23 | 0.46     | 1.88        | 3      | 1     |
| 1:B:34:GLY:O    | 1:B:38:GLU:HB2  | 0.46     | 2.10        | 6      | 2     |
| 1:B:15:ASP:O    | 1:B:19:LYS:HG3  | 0.46     | 2.10        | 3      | 1     |
| 1:A:21:LEU:HG   | 1:B:44:TRP:CE3  | 0.46     | 2.46        | 4      | 8     |
| 1:B:42:ARG:HD3  | 1:B:42:ARG:O    | 0.46     | 2.10        | 7      | 2     |
| 1:A:24:LEU:N    | 1:A:24:LEU:CD2  | 0.46     | 2.79        | 7      | 2     |
| 1:A:44:TRP:HZ2  | 1:B:30:HIS:O    | 0.46     | 1.93        | 8      | 7     |
| 1:B:43:ARG:O    | 1:B:47:ARG:HG3  | 0.46     | 2.11        | 7      | 5     |
| 1:A:13:ARG:CB   | 1:A:13:ARG:CZ   | 0.46     | 2.93        | 2      | 1     |
| 1:A:8:VAL:O     | 1:A:8:VAL:HG12  | 0.46     | 2.11        | 2      | 1     |
| 1:A:17:LEU:HD12 | 1:B:17:LEU:CD2  | 0.46     | 2.41        | 3      | 1     |
| 1:A:35:GLN:HG2  | 1:A:36:ARG:HH11 | 0.46     | 1.70        | 7      | 1     |
| 1:A:8:VAL:O     | 1:A:9:ASP:HB2   | 0.46     | 2.10        | 6      | 5     |
| 1:A:24:LEU:HG   | 1:B:10:ILE:HB   | 0.46     | 1.88        | 8      | 3     |
| 1:A:17:LEU:CD2  | 1:B:14:LEU:HD22 | 0.46     | 2.38        | 4      | 1     |
| 1:A:37:LEU:HD12 | 1:B:44:TRP:CD1  | 0.45     | 2.46        | 3      | 8     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:18:GLU:HB2  | 1:B:40:LEU:HD23 | 0.45     | 1.87        | 2      | 1     |
| 1:A:41:LEU:HG   | 1:B:37:LEU:HD13 | 0.45     | 1.88        | 3      | 6     |
| 1:A:24:LEU:HD21 | 1:B:7:ALA:HA    | 0.45     | 1.86        | 8      | 1     |
| 1:A:33:VAL:HB   | 1:B:44:TRP:CZ2  | 0.45     | 2.46        | 8      | 8     |
| 1:A:10:ILE:CD1  | 1:B:20:ALA:HB1  | 0.45     | 2.41        | 5      | 3     |
| 1:A:41:LEU:HG   | 1:B:37:LEU:CG   | 0.45     | 2.40        | 5      | 2     |
| 1:A:10:ILE:CD1  | 1:A:13:ARG:NH1  | 0.45     | 2.80        | 2      | 1     |
| 1:A:24:LEU:HD23 | 1:A:30:HIS:CD2  | 0.45     | 2.47        | 2      | 1     |
| 1:A:17:LEU:HA   | 1:B:13:ARG:NE   | 0.45     | 2.22        | 2      | 1     |
| 1:B:21:LEU:HD11 | 1:B:37:LEU:HD22 | 0.45     | 1.86        | 6      | 1     |
| 1:A:14:LEU:HD23 | 1:B:40:LEU:HD22 | 0.45     | 1.89        | 5      | 1     |
| 1:A:48:ARG:HH22 | 1:B:29:GLY:HA2  | 0.45     | 1.71        | 2      | 1     |
| 1:B:9:ASP:HB2   | 1:B:12:ASP:OD1  | 0.45     | 2.11        | 4      | 2     |
| 1:B:15:ASP:O    | 1:B:19:LYS:HG2  | 0.45     | 2.12        | 1      | 3     |
| 1:B:23:ALA:O    | 1:B:27:GLU:HG3  | 0.45     | 2.12        | 8      | 3     |
| 1:A:17:LEU:HD21 | 1:B:14:LEU:CD2  | 0.45     | 2.42        | 1      | 1     |
| 1:A:17:LEU:HD23 | 1:B:40:LEU:HD23 | 0.45     | 1.88        | 5      | 1     |
| 1:A:20:ALA:O    | 1:A:24:LEU:HD23 | 0.45     | 2.12        | 8      | 2     |
| 1:A:10:ILE:CG1  | 1:A:13:ARG:NH1  | 0.44     | 2.80        | 2      | 1     |
| 1:A:14:LEU:CG   | 1:B:17:LEU:HD11 | 0.44     | 2.41        | 4      | 1     |
| 1:A:13:ARG:HD3  | 1:B:17:LEU:HA   | 0.44     | 1.89        | 1      | 1     |
| 1:A:13:ARG:NE   | 1:B:17:LEU:HA   | 0.44     | 2.28        | 2      | 1     |
| 1:A:10:ILE:HD13 | 1:B:24:LEU:HD12 | 0.44     | 1.89        | 4      | 1     |
| 1:A:13:ARG:NH1  | 1:B:16:GLU:HB3  | 0.44     | 2.28        | 1      | 1     |
| 1:A:17:LEU:HD23 | 1:B:17:LEU:CD2  | 0.44     | 2.43        | 6      | 1     |
| 1:A:41:LEU:HD23 | 1:B:37:LEU:HD23 | 0.43     | 1.90        | 6      | 1     |
| 1:A:33:VAL:CG2  | 1:B:10:ILE:HG21 | 0.43     | 2.41        | 1      | 1     |
| 1:A:11:GLY:HA2  | 1:A:14:LEU:HD12 | 0.43     | 1.89        | 7      | 1     |
| 1:A:7:ALA:H     | 1:B:20:ALA:HB1  | 0.43     | 1.73        | 4      | 1     |
| 1:B:19:LYS:HA   | 1:B:22:GLU:OE1  | 0.43     | 2.13        | 6      | 2     |
| 1:A:20:ALA:HB2  | 1:B:13:ARG:NH1  | 0.43     | 2.25        | 8      | 1     |
| 1:A:43:ARG:O    | 1:A:47:ARG:HG3  | 0.43     | 2.14        | 2      | 4     |
| 1:A:10:ILE:HD12 | 1:A:13:ARG:NH1  | 0.43     | 2.28        | 2      | 1     |
| 1:A:36:ARG:NH1  | 1:B:11:GLY:HA3  | 0.43     | 2.29        | 2      | 1     |
| 1:A:7:ALA:HB2   | 1:B:24:LEU:HD11 | 0.43     | 1.89        | 8      | 1     |
| 1:A:21:LEU:O    | 1:A:25:SER:N    | 0.43     | 2.51        | 6      | 7     |
| 1:B:10:ILE:HG23 | 1:B:11:GLY:N    | 0.43     | 2.28        | 2      | 1     |
| 1:A:21:LEU:O    | 1:A:24:LEU:N    | 0.43     | 2.52        | 8      | 3     |
| 1:A:10:ILE:HD13 | 1:B:24:LEU:HD13 | 0.43     | 1.91        | 7      | 1     |
| 1:B:27:GLU:HB2  | 1:B:30:HIS:NE2  | 0.43     | 2.29        | 2      | 1     |
| 1:A:10:ILE:HG13 | 1:A:13:ARG:HH12 | 0.43     | 1.74        | 2      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:24:LEU:HD23 | 1:A:30:HIS:CG   | 0.43     | 2.49        | 1      | 2     |
| 1:A:47:ARG:HD3  | 1:B:25:SER:CB   | 0.43     | 2.42        | 7      | 2     |
| 1:A:17:LEU:HD22 | 1:B:13:ARG:HB2  | 0.43     | 1.90        | 7      | 1     |
| 1:A:34:GLY:HA2  | 1:A:37:LEU:HB2  | 0.43     | 1.90        | 1      | 4     |
| 1:B:10:ILE:HD12 | 1:B:13:ARG:NH1  | 0.43     | 2.29        | 2      | 1     |
| 1:B:21:LEU:HD11 | 1:B:33:VAL:HG11 | 0.43     | 1.91        | 1      | 2     |
| 1:A:17:LEU:HD22 | 1:B:17:LEU:CD2  | 0.43     | 2.44        | 8      | 1     |
| 1:A:21:LEU:HD21 | 1:A:37:LEU:HD11 | 0.43     | 1.91        | 5      | 1     |
| 1:A:13:ARG:NH2  | 1:B:17:LEU:CG   | 0.43     | 2.80        | 2      | 1     |
| 1:A:17:LEU:HD22 | 1:B:17:LEU:HD12 | 0.43     | 1.89        | 1      | 1     |
| 1:A:13:ARG:NE   | 1:B:20:ALA:HB2  | 0.43     | 2.29        | 1      | 1     |
| 1:A:40:LEU:HD21 | 1:B:14:LEU:O    | 0.43     | 2.14        | 4      | 1     |
| 1:B:8:VAL:HG12  | 1:B:13:ARG:HG2  | 0.42     | 1.91        | 5      | 2     |
| 1:A:44:TRP:CD2  | 1:B:21:LEU:HD23 | 0.42     | 2.49        | 2      | 2     |
| 1:A:10:ILE:O    | 1:A:13:ARG:HB2  | 0.42     | 2.14        | 5      | 2     |
| 1:A:41:LEU:C    | 1:A:43:ARG:N    | 0.42     | 2.72        | 8      | 5     |
| 1:A:16:GLU:O    | 1:B:13:ARG:NH1  | 0.42     | 2.52        | 8      | 1     |
| 1:A:40:LEU:CB   | 1:B:37:LEU:HD21 | 0.42     | 2.44        | 4      | 2     |
| 1:A:24:LEU:HD23 | 1:A:30:HIS:CE1  | 0.42     | 2.50        | 6      | 3     |
| 1:A:13:ARG:NH2  | 1:B:21:LEU:CD1  | 0.42     | 2.82        | 2      | 1     |
| 1:A:13:ARG:HA   | 1:A:13:ARG:HE   | 0.42     | 1.73        | 5      | 1     |
| 1:B:21:LEU:N    | 1:B:21:LEU:HD23 | 0.42     | 2.30        | 8      | 2     |
| 1:A:24:LEU:HA   | 1:A:27:GLU:HG3  | 0.42     | 1.89        | 2      | 1     |
| 1:A:14:LEU:HD23 | 1:B:40:LEU:CD1  | 0.42     | 2.43        | 7      | 2     |
| 1:A:8:VAL:C     | 1:A:10:ILE:N    | 0.42     | 2.74        | 2      | 1     |
| 1:A:17:LEU:HD23 | 1:B:17:LEU:HD23 | 0.42     | 1.90        | 6      | 1     |
| 1:A:17:LEU:HD23 | 1:A:17:LEU:O    | 0.42     | 2.15        | 3      | 1     |
| 1:A:8:VAL:HG13  | 1:A:8:VAL:O     | 0.42     | 2.15        | 4      | 2     |
| 1:A:17:LEU:HG   | 1:B:17:LEU:HD22 | 0.42     | 1.92        | 2      | 1     |
| 1:A:14:LEU:O    | 1:A:17:LEU:HB3  | 0.42     | 2.15        | 6      | 1     |
| 1:A:19:LYS:HD2  | 1:A:22:GLU:OE2  | 0.42     | 2.15        | 8      | 1     |
| 1:B:17:LEU:O    | 1:B:21:LEU:HD13 | 0.41     | 2.15        | 1      | 1     |
| 1:A:14:LEU:HD13 | 1:B:36:ARG:CB   | 0.41     | 2.45        | 3      | 1     |
| 1:A:8:VAL:O     | 1:A:8:VAL:HG13  | 0.41     | 2.15        | 7      | 1     |
| 1:B:8:VAL:O     | 1:B:9:ASP:CB    | 0.41     | 2.68        | 5      | 1     |
| 1:A:13:ARG:HE   | 1:A:13:ARG:HA   | 0.41     | 1.74        | 6      | 1     |
| 1:A:7:ALA:HA    | 1:B:24:LEU:HD21 | 0.41     | 1.93        | 6      | 1     |
| 1:A:40:LEU:CD1  | 1:B:37:LEU:HD11 | 0.41     | 2.45        | 6      | 1     |
| 1:A:44:TRP:HE1  | 1:B:34:GLY:N    | 0.41     | 2.12        | 1      | 1     |
| 1:A:13:ARG:CB   | 1:B:17:LEU:HG   | 0.41     | 2.46        | 1      | 1     |
| 1:B:24:LEU:HD12 | 1:B:30:HIS:CE1  | 0.41     | 2.50        | 6      | 1     |

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| Atom-1          | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|-----------------|-----------------|----------|-------------|--------|-------|
|                 |                 |          |             | Worst  | Total |
| 1:A:45:ASN:O    | 1:A:48:ARG:HB2  | 0.41     | 2.16        | 3      | 1     |
| 1:B:24:LEU:CD2  | 1:B:24:LEU:N    | 0.41     | 2.83        | 5      | 1     |
| 1:A:48:ARG:HH12 | 1:B:30:HIS:N    | 0.41     | 2.14        | 3      | 1     |
| 1:A:24:LEU:HD12 | 1:A:30:HIS:CE1  | 0.41     | 2.51        | 4      | 1     |
| 1:B:24:LEU:N    | 1:B:24:LEU:CD2  | 0.41     | 2.83        | 6      | 1     |
| 1:A:41:LEU:CG   | 1:B:37:LEU:HD13 | 0.41     | 2.45        | 3      | 1     |
| 1:A:10:ILE:HG23 | 1:A:11:GLY:N    | 0.41     | 2.30        | 8      | 1     |
| 1:A:17:LEU:HD23 | 1:B:17:LEU:HD12 | 0.41     | 1.91        | 1      | 1     |
| 1:A:8:VAL:O     | 1:A:9:ASP:HB3   | 0.41     | 2.16        | 5      | 2     |
| 1:A:40:LEU:HD13 | 1:B:17:LEU:CD2  | 0.41     | 2.37        | 2      | 1     |
| 1:A:24:LEU:HD22 | 1:B:10:ILE:CB   | 0.41     | 2.46        | 3      | 2     |
| 1:A:20:ALA:CB   | 1:B:13:ARG:HG3  | 0.41     | 2.46        | 3      | 1     |
| 1:A:17:LEU:HD22 | 1:B:17:LEU:HD22 | 0.41     | 1.92        | 8      | 1     |
| 1:A:13:ARG:NH1  | 1:B:16:GLU:O    | 0.41     | 2.54        | 8      | 1     |
| 1:A:10:ILE:HD12 | 1:A:10:ILE:HA   | 0.41     | 1.78        | 4      | 1     |
| 1:A:14:LEU:CD2  | 1:B:17:LEU:HD21 | 0.41     | 2.46        | 3      | 1     |
| 1:A:7:ALA:HB2   | 1:B:24:LEU:HD21 | 0.40     | 1.93        | 5      | 1     |
| 1:B:42:ARG:C    | 1:B:42:ARG:HD3  | 0.40     | 2.37        | 6      | 1     |
| 1:A:41:LEU:O    | 1:A:42:ARG:C    | 0.40     | 2.60        | 7      | 2     |
| 1:A:24:LEU:HG   | 1:B:10:ILE:CG1  | 0.40     | 2.46        | 7      | 1     |
| 1:A:42:ARG:C    | 1:A:42:ARG:HD3  | 0.40     | 2.36        | 6      | 1     |

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

| Mol | Chain | Analysed      | Favoured     | Allowed    | Outliers   | Percentiles |    |
|-----|-------|---------------|--------------|------------|------------|-------------|----|
| 1   | A     | 43/60 (72%)   | 36±1 (84±2%) | 4±1 (9±2%) | 3±0 (7±1%) | 3           | 19 |
| 1   | B     | 43/60 (72%)   | 37±1 (86±1%) | 4±0 (8±1%) | 2±1 (5±2%) | 5           | 25 |
| All | All   | 688/960 (72%) | 587 (85%)    | 60 (9%)    | 41 (6%)    | 4           | 21 |

All 6 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     | 10  | ILE  | 8              |
| 1   | A     | 25  | SER  | 8              |
| 1   | B     | 25  | SER  | 8              |
| 1   | A     | 8   | VAL  | 7              |
| 1   | B     | 10  | ILE  | 5              |
| 1   | B     | 8   | VAL  | 5              |

### 6.3.2 Protein sidechains [i](#)

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

| Mol | Chain | Analysed      | Rotameric    | Outliers   | Percentiles |    |
|-----|-------|---------------|--------------|------------|-------------|----|
| 1   | A     | 35/47 (74%)   | 33±1 (94±3%) | 2±1 (6±3%) | 26          | 72 |
| 1   | B     | 35/47 (74%)   | 34±0 (97±1%) | 1±0 (3±1%) | 50          | 89 |
| All | All   | 560/752 (74%) | 533 (95%)    | 27 (5%)    | 36          | 80 |

All 10 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     | 21  | LEU  | 8              |
| 1   | B     | 37  | LEU  | 6              |
| 1   | A     | 17  | LEU  | 3              |
| 1   | A     | 35  | GLN  | 3              |
| 1   | A     | 12  | ASP  | 2              |
| 1   | B     | 13  | ARG  | 1              |
| 1   | B     | 42  | ARG  | 1              |
| 1   | B     | 17  | LEU  | 1              |
| 1   | A     | 42  | ARG  | 1              |
| 1   | A     | 13  | ARG  | 1              |

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 74% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5885

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                  | 2358 |
| Number of shifts mapped to atoms        | 1136 |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 1222 |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

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

- Residue not found in structure. All 1222 occurrences are reported below.

| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 112 | ARG  | HB3  | 1.9968     | 0.02        | 1         |
| A     | 98  | LYS  | HA   | 3.8503     | 0.02        | 1         |
| A     | 74  | PHE  | CA   | 55.606     | 0.05        | 1         |
| A     | 116 | HIS  | CA   | 56.424     | 0.05        | 1         |
| A     | 118 | ALA  | HB1  | 1.454      | 0.02        | 1         |
| A     | 72  | GLN  | CB   | 28.911     | 0.05        | 1         |
| A     | 84  | GLY  | H    | 8.436      | 0.02        | 1         |
| B     | 105 | ASP  | H    | 9.0481     | 0.02        | 1         |
| B     | 102 | THR  | HA   | 4.041      | 0.02        | 1         |
| A     | 86  | ASN  | HB2  | 2.86       | 0.02        | 1         |
| A     | 61  | ALA  | HB3  | 1.3784     | 0.02        | 1         |
| A     | 81  | LEU  | CB   | 41.926     | 0.05        | 1         |
| A     | 79  | ASP  | N    | 120.011    | 0.05        | 1         |
| B     | 110 | ARG  | HA   | 4.16       | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 91  | GLU  | HA   | 4.1593     | 0.02        | 1         |
| B     | 108 | THR  | C    | 176.228    | 0.05        | 1         |
| A     | 111 | LEU  | HD21 | 1.0021     | 0.02        | 1         |
| A     | 103 | GLU  | HG2  | 2.457      | 0.02        | 2         |
| B     | 118 | ALA  | H    | 8.2797     | 0.02        | 1         |
| A     | 89  | THR  | N    | 118.985    | 0.05        | 1         |
| A     | 118 | ALA  | H    | 8.2797     | 0.02        | 1         |
| A     | 96  | TYR  | CE1  | 118.4737   | 0.05        | 1         |
| A     | 101 | VAL  | CA   | 67.467     | 0.05        | 1         |
| B     | 102 | THR  | HG23 | 1.2612     | 0.02        | 1         |
| B     | 81  | LEU  | CB   | 41.926     | 0.05        | 1         |
| B     | 62  | SER  | HB3  | 3.9317     | 0.02        | 2         |
| A     | 69  | MET  | C    | 179.38     | 0.05        | 1         |
| B     | 87  | GLY  | HA2  | 4.0        | 0.02        | 1         |
| B     | 62  | SER  | HA   | 4.3888     | 0.02        | 1         |
| A     | 74  | PHE  | C    | 177.153    | 0.05        | 1         |
| B     | 85  | ASP  | HB2  | 2.692      | 0.02        | 1         |
| B     | 70  | LEU  | CA   | 57.631     | 0.05        | 1         |
| A     | 99  | ARG  | HB2  | 1.699      | 0.02        | 1         |
| B     | 89  | THR  | H    | 8.3848     | 0.02        | 1         |
| A     | 67  | PHE  | CB   | 36.965     | 0.05        | 1         |
| A     | 75  | GLY  | CA   | 45.837     | 0.05        | 1         |
| A     | 74  | PHE  | HB3  | 3.1222     | 0.02        | 2         |
| B     | 115 | GLU  | HA   | 4.122      | 0.02        | 1         |
| A     | 101 | VAL  | HG12 | 1.1774     | 0.02        | 2         |
| A     | 92  | LYS  | N    | 120.484    | 0.05        | 1         |
| A     | 109 | ALA  | N    | 123.276    | 0.05        | 1         |
| A     | 63  | ASP  | CA   | 56.654     | 0.05        | 1         |
| B     | 114 | VAL  | CB   | 32.09      | 0.05        | 1         |
| A     | 67  | PHE  | CZ   | 128.068    | 0.05        | 1         |
| A     | 94  | ARG  | C    | 178.078    | 0.05        | 1         |
| B     | 111 | LEU  | HD22 | 1.0021     | 0.02        | 1         |
| A     | 117 | ARG  | C    | 176.277    | 0.05        | 1         |
| A     | 88  | MET  | HB3  | 2.1355     | 0.02        | 2         |
| A     | 75  | GLY  | C    | 174.75     | 0.05        | 1         |
| A     | 85  | ASP  | H    | 8.212      | 0.02        | 1         |
| A     | 100 | THR  | CA   | 67.753     | 0.05        | 1         |
| A     | 93  | LEU  | HA   | 4.1277     | 0.02        | 1         |
| A     | 109 | ALA  | HB3  | 1.5713     | 0.02        | 1         |
| B     | 100 | THR  | HB   | 3.9695     | 0.02        | 1         |
| B     | 67  | PHE  | HE1  | 7.0507     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 83  | SER  | HB2  | 3.92       | 0.02        | 1         |
| B     | 66  | LEU  | HG   | 1.54       | 0.02        | 1         |
| A     | 73  | ARG  | CG   | 27.482     | 0.05        | 1         |
| B     | 74  | PHE  | HE2  | 7.3494     | 0.02        | 1         |
| B     | 102 | THR  | CG2  | 21.7015    | 0.05        | 1         |
| B     | 68  | SER  | HA   | 4.3372     | 0.02        | 1         |
| A     | 105 | ASP  | H    | 9.0481     | 0.02        | 1         |
| B     | 117 | ARG  | N    | 120.851    | 0.05        | 1         |
| A     | 114 | VAL  | HG11 | 1.0836     | 0.02        | 2         |
| B     | 93  | LEU  | HB2  | 2.2778     | 0.02        | 2         |
| B     | 66  | LEU  | HB2  | 1.521      | 0.02        | 1         |
| A     | 107 | VAL  | HG22 | 1.0954     | 0.02        | 2         |
| A     | 74  | PHE  | CE1  | 129.082    | 0.05        | 1         |
| B     | 76  | GLY  | CA   | 45.48      | 0.05        | 1         |
| B     | 117 | ARG  | HB3  | 1.8478     | 0.02        | 2         |
| B     | 104 | LEU  | CD2  | 23.058     | 0.05        | 2         |
| A     | 83  | SER  | CA   | 58.593     | 0.05        | 1         |
| B     | 73  | ARG  | HA   | 4.0762     | 0.02        | 1         |
| A     | 115 | GLU  | CB   | 30.154     | 0.05        | 1         |
| A     | 74  | PHE  | CD1  | 131.005    | 0.05        | 1         |
| B     | 89  | THR  | CB   | 69.004     | 0.05        | 1         |
| B     | 67  | PHE  | CB   | 36.965     | 0.05        | 1         |
| A     | 70  | LEU  | CB   | 40.583     | 0.05        | 1         |
| B     | 101 | VAL  | HG12 | 1.1774     | 0.02        | 2         |
| B     | 104 | LEU  | HA   | 4.1554     | 0.02        | 1         |
| A     | 98  | LYS  | H    | 8.4272     | 0.02        | 1         |
| A     | 94  | ARG  | HG2  | 1.524      | 0.02        | 1         |
| A     | 120 | GLU  | H    | 7.868      | 0.02        | 1         |
| B     | 67  | PHE  | CZ   | 128.068    | 0.05        | 1         |
| A     | 106 | SER  | CA   | 61.691     | 0.05        | 1         |
| B     | 74  | PHE  | CB   | 38.827     | 0.05        | 1         |
| B     | 104 | LEU  | HB3  | 1.4968     | 0.02        | 2         |
| B     | 115 | GLU  | HB2  | 1.985      | 0.02        | 1         |
| B     | 99  | ARG  | HB2  | 1.699      | 0.02        | 1         |
| B     | 107 | VAL  | HA   | 3.8852     | 0.02        | 1         |
| A     | 82  | MET  | HB3  | 2.027      | 0.02        | 2         |
| A     | 75  | GLY  | N    | 127.302    | 0.05        | 1         |
| B     | 61  | ALA  | CB   | 19.203     | 0.05        | 1         |
| B     | 106 | SER  | H    | 8.1317     | 0.02        | 1         |
| B     | 86  | ASN  | H    | 8.507      | 0.02        | 1         |
| B     | 110 | ARG  | HD3  | 3.2473     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 95  | ARG  | H    | 8.3875     | 0.02        | 1         |
| A     | 65  | GLU  | HA   | 4.0222     | 0.02        | 1         |
| A     | 96  | TYR  | CD1  | 132.505    | 0.05        | 1         |
| B     | 104 | LEU  | CG   | 27.402     | 0.05        | 1         |
| A     | 102 | THR  | CB   | 68.584     | 0.05        | 1         |
| A     | 91  | GLU  | H    | 7.618      | 0.02        | 1         |
| B     | 79  | ASP  | C    | 176.446    | 0.05        | 1         |
| A     | 113 | GLU  | C    | 178.913    | 0.05        | 1         |
| A     | 83  | SER  | C    | 175.04     | 0.05        | 1         |
| A     | 72  | GLN  | HG3  | 2.416      | 0.02        | 2         |
| A     | 79  | ASP  | CB   | 40.68      | 0.05        | 1         |
| A     | 93  | LEU  | H    | 8.6177     | 0.02        | 1         |
| B     | 86  | ASN  | HB3  | 2.86       | 0.02        | 1         |
| B     | 61  | ALA  | HB3  | 1.3784     | 0.02        | 1         |
| B     | 93  | LEU  | HA   | 4.1277     | 0.02        | 1         |
| B     | 78  | GLU  | CB   | 30.027     | 0.05        | 1         |
| A     | 103 | GLU  | HB2  | 2.024      | 0.02        | 1         |
| B     | 63  | ASP  | C    | 176.199    | 0.05        | 1         |
| B     | 73  | ARG  | CG   | 27.482     | 0.05        | 1         |
| A     | 102 | THR  | HG22 | 1.2612     | 0.02        | 1         |
| B     | 72  | GLN  | HE21 | 7.434      | 0.02        | 2         |
| B     | 75  | GLY  | HA2  | 4.254      | 0.02        | 2         |
| A     | 79  | ASP  | HA   | 4.5162     | 0.02        | 1         |
| A     | 74  | PHE  | H    | 8.3558     | 0.02        | 1         |
| B     | 74  | PHE  | H    | 8.3558     | 0.02        | 1         |
| A     | 100 | THR  | HA   | 4.3533     | 0.02        | 1         |
| A     | 67  | PHE  | HB3  | 2.9777     | 0.02        | 2         |
| A     | 62  | SER  | C    | 175.38     | 0.05        | 1         |
| A     | 97  | LEU  | HD13 | 1.0221     | 0.02        | 1         |
| A     | 88  | MET  | HG3  | 2.5652     | 0.02        | 2         |
| A     | 114 | VAL  | HG23 | 0.9746     | 0.02        | 2         |
| A     | 116 | HIS  | HB2  | 3.3644     | 0.02        | 2         |
| B     | 88  | MET  | HB3  | 2.1355     | 0.02        | 2         |
| A     | 97  | LEU  | CD2  | 27.251     | 0.05        | 1         |
| B     | 68  | SER  | C    | 177.344    | 0.05        | 1         |
| B     | 61  | ALA  | H    | 8.278      | 0.02        | 1         |
| B     | 68  | SER  | CA   | 61.769     | 0.05        | 1         |
| A     | 62  | SER  | HB3  | 3.9317     | 0.02        | 2         |
| A     | 79  | ASP  | HB3  | 2.594      | 0.02        | 2         |
| A     | 85  | ASP  | C    | 176.308    | 0.05        | 1         |
| A     | 113 | GLU  | HB3  | 2.247      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 114 | VAL  | HG21 | 0.9746     | 0.02        | 2         |
| B     | 108 | THR  | HG23 | 1.3239     | 0.02        | 1         |
| B     | 111 | LEU  | HD12 | 1.0021     | 0.02        | 1         |
| B     | 93  | LEU  | HD23 | 0.93       | 0.02        | 2         |
| A     | 114 | VAL  | H    | 8.033      | 0.02        | 1         |
| B     | 90  | GLU  | HB3  | 2.0393     | 0.02        | 2         |
| A     | 89  | THR  | HG21 | 1.2918     | 0.02        | 1         |
| A     | 65  | GLU  | HG3  | 2.22       | 0.02        | 2         |
| A     | 84  | GLY  | HA3  | 3.99       | 0.02        | 1         |
| B     | 67  | PHE  | HB2  | 3.1709     | 0.02        | 2         |
| B     | 77  | GLY  | N    | 127.741    | 0.05        | 1         |
| B     | 111 | LEU  | H    | 8.4697     | 0.02        | 1         |
| A     | 110 | ARG  | HB3  | 2.0495     | 0.02        | 1         |
| A     | 94  | ARG  | H    | 8.3326     | 0.02        | 1         |
| A     | 111 | LEU  | HD11 | 1.0021     | 0.02        | 1         |
| B     | 90  | GLU  | HG2  | 2.1665     | 0.02        | 1         |
| A     | 93  | LEU  | C    | 178.605    | 0.05        | 1         |
| B     | 63  | ASP  | CA   | 56.654     | 0.05        | 1         |
| B     | 67  | PHE  | CA   | 58.826     | 0.05        | 1         |
| A     | 104 | LEU  | C    | 179.991    | 0.05        | 1         |
| A     | 109 | ALA  | CB   | 17.809     | 0.05        | 1         |
| B     | 95  | ARG  | HG2  | 1.862      | 0.02        | 2         |
| A     | 104 | LEU  | H    | 8.9435     | 0.02        | 1         |
| A     | 84  | GLY  | N    | 110.24     | 0.05        | 1         |
| B     | 78  | GLU  | H    | 8.504      | 0.02        | 1         |
| B     | 103 | GLU  | C    | 178.219    | 0.05        | 1         |
| B     | 101 | VAL  | HA   | 3.5666     | 0.02        | 1         |
| B     | 69  | MET  | HB3  | 2.2694     | 0.02        | 1         |
| B     | 111 | LEU  | HB3  | 1.5034     | 0.02        | 2         |
| A     | 74  | PHE  | CB   | 38.827     | 0.05        | 1         |
| A     | 66  | LEU  | CA   | 58.092     | 0.05        | 1         |
| B     | 109 | ALA  | HB3  | 1.5713     | 0.02        | 1         |
| A     | 72  | GLN  | CG   | 34.01      | 0.05        | 1         |
| B     | 84  | GLY  | C    | 173.946    | 0.05        | 1         |
| A     | 111 | LEU  | CA   | 58.751     | 0.05        | 1         |
| B     | 77  | GLY  | H    | 8.415      | 0.02        | 1         |
| B     | 117 | ARG  | CB   | 30.615     | 0.05        | 1         |
| B     | 101 | VAL  | CG1  | 24.748     | 0.05        | 2         |
| B     | 114 | VAL  | C    | 178.062    | 0.05        | 1         |
| B     | 81  | LEU  | HB3  | 1.5887     | 0.02        | 2         |
| A     | 81  | LEU  | CA   | 55.67      | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 86  | ASN  | N    | 118.739    | 0.05        | 1         |
| A     | 112 | ARG  | N    | 116.931    | 0.05        | 1         |
| A     | 78  | GLU  | CG   | 36.283     | 0.05        | 1         |
| A     | 90  | GLU  | HG3  | 2.1665     | 0.02        | 1         |
| B     | 78  | GLU  | HB2  | 2.059      | 0.02        | 2         |
| A     | 92  | LYS  | HB2  | 1.8253     | 0.02        | 2         |
| B     | 86  | ASN  | HD22 | 6.965      | 0.02        | 1         |
| B     | 108 | THR  | HB   | 4.4064     | 0.02        | 1         |
| B     | 86  | ASN  | C    | 175.824    | 0.05        | 1         |
| B     | 80  | LEU  | HB3  | 1.525      | 0.02        | 2         |
| B     | 113 | GLU  | CG   | 33.981     | 0.05        | 1         |
| A     | 80  | LEU  | HG   | 1.562      | 0.02        | 1         |
| B     | 97  | LEU  | N    | 124.775    | 0.05        | 1         |
| A     | 102 | THR  | CG2  | 21.7015    | 0.05        | 1         |
| B     | 111 | LEU  | CB   | 41.5949    | 0.05        | 1         |
| B     | 89  | THR  | N    | 118.985    | 0.05        | 1         |
| A     | 117 | ARG  | HD2  | 3.244      | 0.02        | 1         |
| B     | 117 | ARG  | HA   | 4.2938     | 0.02        | 1         |
| A     | 70  | LEU  | N    | 121.809    | 0.05        | 1         |
| A     | 96  | TYR  | CE2  | 118.4737   | 0.05        | 1         |
| A     | 72  | GLN  | C    | 178.127    | 0.05        | 1         |
| A     | 101 | VAL  | CB   | 31.411     | 0.05        | 1         |
| A     | 109 | ALA  | H    | 7.9484     | 0.02        | 1         |
| A     | 101 | VAL  | HG21 | 0.9529     | 0.02        | 2         |
| A     | 111 | LEU  | HB3  | 1.5034     | 0.02        | 2         |
| A     | 104 | LEU  | HB2  | 2.4038     | 0.02        | 2         |
| A     | 117 | ARG  | N    | 120.851    | 0.05        | 1         |
| B     | 63  | ASP  | N    | 122.743    | 0.05        | 1         |
| B     | 105 | ASP  | HB3  | 2.6896     | 0.02        | 2         |
| B     | 61  | ALA  | N    | 124.679    | 0.05        | 1         |
| A     | 108 | THR  | CA   | 67.738     | 0.05        | 1         |
| A     | 93  | LEU  | HB2  | 2.2778     | 0.02        | 2         |
| B     | 62  | SER  | CA   | 58.466     | 0.05        | 1         |
| A     | 87  | GLY  | C    | 177.446    | 0.05        | 1         |
| B     | 114 | VAL  | CA   | 64.696     | 0.05        | 1         |
| B     | 88  | MET  | HG3  | 2.5652     | 0.02        | 2         |
| B     | 116 | HIS  | C    | 175.353    | 0.05        | 1         |
| A     | 119 | GLY  | C    | 173.361    | 0.05        | 1         |
| A     | 115 | GLU  | HG2  | 2.4338     | 0.02        | 2         |
| B     | 114 | VAL  | HG22 | 0.9746     | 0.02        | 2         |
| B     | 87  | GLY  | CA   | 45.746     | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 65  | GLU  | CA   | 59.112     | 0.05        | 1         |
| B     | 73  | ARG  | HG2  | 1.809      | 0.02        | 1         |
| B     | 117 | ARG  | H    | 8.101      | 0.02        | 1         |
| A     | 101 | VAL  | HA   | 3.5666     | 0.02        | 1         |
| B     | 112 | ARG  | C    | 178.907    | 0.05        | 1         |
| B     | 74  | PHE  | CE2  | 129.082    | 0.05        | 1         |
| B     | 107 | VAL  | N    | 120.402    | 0.05        | 1         |
| A     | 111 | LEU  | HB2  | 2.141      | 0.02        | 2         |
| A     | 66  | LEU  | N    | 122.23     | 0.05        | 1         |
| A     | 113 | GLU  | HG3  | 2.4697     | 0.02        | 2         |
| A     | 95  | ARG  | HB3  | 1.855      | 0.02        | 1         |
| B     | 104 | LEU  | HD21 | 0.9838     | 0.02        | 2         |
| A     | 74  | PHE  | CE2  | 129.082    | 0.05        | 1         |
| A     | 112 | ARG  | CA   | 59.108     | 0.05        | 1         |
| B     | 113 | GLU  | HA   | 4.1707     | 0.02        | 1         |
| A     | 112 | ARG  | HB2  | 1.9968     | 0.02        | 1         |
| B     | 110 | ARG  | CD   | 43.36      | 0.05        | 1         |
| A     | 93  | LEU  | CB   | 44.045     | 0.05        | 1         |
| A     | 111 | LEU  | HD13 | 1.0021     | 0.02        | 1         |
| A     | 91  | GLU  | C    | 178.68     | 0.05        | 1         |
| B     | 89  | THR  | HG23 | 1.2918     | 0.02        | 1         |
| B     | 97  | LEU  | HD23 | 1.0221     | 0.02        | 1         |
| A     | 78  | GLU  | HA   | 4.2436     | 0.02        | 1         |
| B     | 97  | LEU  | CA   | 59.0       | 0.05        | 1         |
| A     | 90  | GLU  | N    | 120.081    | 0.05        | 1         |
| A     | 70  | LEU  | CA   | 57.631     | 0.05        | 1         |
| A     | 107 | VAL  | HG12 | 1.2189     | 0.02        | 2         |
| B     | 67  | PHE  | CE2  | 130.187    | 0.05        | 1         |
| B     | 92  | LYS  | HB3  | 1.709      | 0.02        | 2         |
| A     | 108 | THR  | HB   | 4.4064     | 0.02        | 1         |
| B     | 63  | ASP  | HB3  | 2.2455     | 0.02        | 2         |
| B     | 70  | LEU  | H    | 8.3178     | 0.02        | 1         |
| A     | 93  | LEU  | HD13 | 1.0569     | 0.02        | 2         |
| B     | 64  | ASP  | N    | 116.823    | 0.05        | 1         |
| A     | 65  | GLU  | N    | 119.941    | 0.05        | 1         |
| A     | 106 | SER  | CB   | 62.755     | 0.05        | 1         |
| A     | 120 | GLU  | N    | 125.138    | 0.05        | 1         |
| A     | 70  | LEU  | CD2  | 21.72      | 0.05        | 2         |
| A     | 107 | VAL  | CA   | 66.377     | 0.05        | 1         |
| A     | 113 | GLU  | H    | 7.711      | 0.02        | 1         |
| B     | 92  | LYS  | N    | 120.484    | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 87  | GLY  | N    | 127.57     | 0.05        | 1         |
| B     | 104 | LEU  | CB   | 41.847     | 0.05        | 1         |
| B     | 85  | ASP  | CB   | 41.217     | 0.05        | 1         |
| B     | 96  | TYR  | CB   | 38.15      | 0.05        | 1         |
| A     | 118 | ALA  | C    | 178.096    | 0.05        | 1         |
| A     | 69  | MET  | HA   | 4.1346     | 0.02        | 1         |
| A     | 95  | ARG  | H    | 8.3875     | 0.02        | 1         |
| B     | 65  | GLU  | N    | 119.941    | 0.05        | 1         |
| A     | 87  | GLY  | HA3  | 4.0        | 0.02        | 1         |
| B     | 90  | GLU  | CA   | 60.941     | 0.05        | 1         |
| B     | 95  | ARG  | HB3  | 1.855      | 0.02        | 1         |
| A     | 103 | GLU  | HA   | 4.1932     | 0.02        | 1         |
| A     | 110 | ARG  | HG2  | 1.483      | 0.02        | 1         |
| B     | 103 | GLU  | HB2  | 2.024      | 0.02        | 1         |
| B     | 72  | GLN  | CG   | 34.01      | 0.05        | 1         |
| B     | 109 | ALA  | N    | 123.276    | 0.05        | 1         |
| A     | 63  | ASP  | H    | 8.5392     | 0.02        | 1         |
| B     | 74  | PHE  | CE1  | 129.082    | 0.05        | 1         |
| B     | 78  | GLU  | CG   | 36.283     | 0.05        | 1         |
| B     | 63  | ASP  | HA   | 4.0461     | 0.02        | 1         |
| B     | 73  | ARG  | CB   | 30.439     | 0.05        | 1         |
| B     | 83  | SER  | C    | 175.04     | 0.05        | 1         |
| B     | 107 | VAL  | CG2  | 22.209     | 0.05        | 2         |
| B     | 67  | PHE  | HD1  | 6.6752     | 0.02        | 1         |
| B     | 110 | ARG  | HB2  | 2.0495     | 0.02        | 1         |
| B     | 98  | LYS  | H    | 8.4272     | 0.02        | 1         |
| B     | 67  | PHE  | HB3  | 2.9777     | 0.02        | 2         |
| A     | 80  | LEU  | HB3  | 1.525      | 0.02        | 2         |
| A     | 77  | GLY  | HA2  | 4.0045     | 0.02        | 1         |
| B     | 103 | GLU  | HG2  | 2.457      | 0.02        | 2         |
| A     | 85  | ASP  | HB2  | 2.692      | 0.02        | 1         |
| A     | 70  | LEU  | HD21 | 0.8188     | 0.02        | 2         |
| A     | 76  | GLY  | HA3  | 3.975      | 0.02        | 2         |
| B     | 105 | ASP  | N    | 123.415    | 0.05        | 1         |
| A     | 61  | ALA  | N    | 124.679    | 0.05        | 1         |
| B     | 107 | VAL  | HG13 | 1.2189     | 0.02        | 2         |
| A     | 78  | GLU  | C    | 176.451    | 0.05        | 1         |
| B     | 93  | LEU  | H    | 8.6177     | 0.02        | 1         |
| A     | 78  | GLU  | H    | 8.504      | 0.02        | 1         |
| B     | 107 | VAL  | HG22 | 1.0954     | 0.02        | 2         |
| A     | 104 | LEU  | HD12 | 1.1055     | 0.02        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 65  | GLU  | CA   | 59.112     | 0.05        | 1         |
| B     | 92  | LYS  | C    | 178.68     | 0.05        | 1         |
| A     | 80  | LEU  | C    | 177.403    | 0.05        | 1         |
| B     | 86  | ASN  | HD21 | 7.648      | 0.02        | 1         |
| A     | 86  | ASN  | HD22 | 6.965      | 0.02        | 1         |
| A     | 107 | VAL  | N    | 120.402    | 0.05        | 1         |
| A     | 88  | MET  | H    | 8.2253     | 0.02        | 1         |
| A     | 104 | LEU  | HD23 | 0.9838     | 0.02        | 2         |
| B     | 96  | TYR  | C    | 179.519    | 0.05        | 1         |
| B     | 96  | TYR  | HB3  | 2.9381     | 0.02        | 2         |
| A     | 71  | ASP  | CA   | 57.618     | 0.05        | 1         |
| B     | 63  | ASP  | CB   | 39.686     | 0.05        | 1         |
| B     | 63  | ASP  | HB2  | 2.4453     | 0.02        | 2         |
| B     | 100 | THR  | C    | 176.489    | 0.05        | 1         |
| A     | 115 | GLU  | C    | 177.308    | 0.05        | 1         |
| A     | 69  | MET  | N    | 121.599    | 0.05        | 1         |
| B     | 117 | ARG  | HG3  | 1.72       | 0.02        | 1         |
| A     | 116 | HIS  | H    | 8.065      | 0.02        | 1         |
| A     | 67  | PHE  | HA   | 4.1112     | 0.02        | 1         |
| B     | 71  | ASP  | HB2  | 2.945      | 0.02        | 2         |
| A     | 68  | SER  | HB3  | 3.9998     | 0.02        | 1         |
| A     | 102 | THR  | H    | 7.8492     | 0.02        | 1         |
| B     | 68  | SER  | HB2  | 3.9998     | 0.02        | 1         |
| B     | 108 | THR  | HG22 | 1.3239     | 0.02        | 1         |
| A     | 103 | GLU  | N    | 122.544    | 0.05        | 1         |
| B     | 76  | GLY  | N    | 127.652    | 0.05        | 1         |
| A     | 90  | GLU  | C    | 176.85     | 0.05        | 1         |
| A     | 80  | LEU  | CA   | 55.592     | 0.05        | 1         |
| A     | 97  | LEU  | C    | 177.683    | 0.05        | 1         |
| B     | 70  | LEU  | HD22 | 0.8188     | 0.02        | 2         |
| A     | 107 | VAL  | CG1  | 22.534     | 0.05        | 2         |
| A     | 111 | LEU  | CD2  | 26.404     | 0.05        | 1         |
| B     | 111 | LEU  | HD13 | 1.0021     | 0.02        | 1         |
| B     | 65  | GLU  | HB3  | 2.0165     | 0.02        | 2         |
| A     | 90  | GLU  | HB2  | 2.2598     | 0.02        | 2         |
| A     | 83  | SER  | HA   | 4.4163     | 0.02        | 1         |
| B     | 88  | MET  | CG   | 32.3075    | 0.05        | 1         |
| B     | 96  | TYR  | CE2  | 118.4737   | 0.05        | 1         |
| A     | 103 | GLU  | CA   | 58.964     | 0.05        | 1         |
| B     | 72  | GLN  | HB3  | 2.0145     | 0.02        | 2         |
| B     | 69  | MET  | HG2  | 2.7392     | 0.02        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 102 | THR  | HB   | 4.2957     | 0.02        | 1         |
| B     | 96  | TYR  | HD2  | 7.2139     | 0.02        | 1         |
| A     | 79  | ASP  | C    | 176.446    | 0.05        | 1         |
| B     | 110 | ARG  | HG3  | 1.483      | 0.02        | 1         |
| B     | 113 | GLU  | CB   | 29.797     | 0.05        | 1         |
| A     | 116 | HIS  | CB   | 28.596     | 0.05        | 1         |
| A     | 70  | LEU  | HD13 | 0.9524     | 0.02        | 2         |
| A     | 90  | GLU  | CB   | 29.8281    | 0.05        | 1         |
| B     | 115 | GLU  | N    | 119.665    | 0.05        | 1         |
| B     | 97  | LEU  | HD13 | 1.0221     | 0.02        | 1         |
| A     | 89  | THR  | CB   | 69.004     | 0.05        | 1         |
| A     | 118 | ALA  | HA   | 4.347      | 0.02        | 1         |
| B     | 119 | GLY  | H    | 8.2435     | 0.02        | 1         |
| B     | 120 | GLU  | N    | 125.138    | 0.05        | 1         |
| B     | 68  | SER  | H    | 8.0576     | 0.02        | 1         |
| B     | 99  | ARG  | C    | 178.589    | 0.05        | 1         |
| B     | 75  | GLY  | H    | 7.9742     | 0.02        | 1         |
| A     | 69  | MET  | CA   | 59.008     | 0.05        | 1         |
| B     | 62  | SER  | C    | 175.38     | 0.05        | 1         |
| A     | 111 | LEU  | HG   | 1.717      | 0.02        | 1         |
| B     | 71  | ASP  | HA   | 4.4852     | 0.02        | 1         |
| B     | 104 | LEU  | N    | 121.08     | 0.05        | 1         |
| A     | 88  | MET  | HB2  | 2.2635     | 0.02        | 2         |
| B     | 65  | GLU  | CB   | 29.5665    | 0.05        | 1         |
| B     | 113 | GLU  | HG3  | 2.4697     | 0.02        | 2         |
| B     | 118 | ALA  | CB   | 19.104     | 0.05        | 1         |
| B     | 79  | ASP  | N    | 120.011    | 0.05        | 1         |
| B     | 66  | LEU  | HA   | 4.0843     | 0.02        | 1         |
| A     | 108 | THR  | CG2  | 21.069     | 0.05        | 1         |
| B     | 96  | TYR  | CD1  | 132.505    | 0.05        | 1         |
| A     | 95  | ARG  | HG2  | 1.862      | 0.02        | 2         |
| A     | 64  | ASP  | C    | 179.052    | 0.05        | 1         |
| B     | 89  | THR  | HA   | 3.9534     | 0.02        | 1         |
| A     | 61  | ALA  | C    | 178.053    | 0.05        | 1         |
| A     | 116 | HIS  | HA   | 4.6413     | 0.02        | 1         |
| B     | 100 | THR  | HG23 | 1.3291     | 0.02        | 1         |
| B     | 73  | ARG  | N    | 119.296    | 0.05        | 1         |
| A     | 91  | GLU  | N    | 116.636    | 0.05        | 1         |
| B     | 111 | LEU  | HA   | 4.1023     | 0.02        | 1         |
| B     | 93  | LEU  | CG   | 27.448     | 0.05        | 1         |
| A     | 92  | LYS  | C    | 178.68     | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 108 | THR  | CG2  | 21.069     | 0.05        | 1         |
| A     | 86  | ASN  | HB3  | 2.86       | 0.02        | 1         |
| A     | 61  | ALA  | HB2  | 1.3784     | 0.02        | 1         |
| B     | 76  | GLY  | HA3  | 3.975      | 0.02        | 2         |
| B     | 67  | PHE  | CD1  | 130.7586   | 0.05        | 1         |
| A     | 119 | GLY  | HA3  | 3.9922     | 0.02        | 1         |
| B     | 73  | ARG  | HB3  | 1.4748     | 0.02        | 2         |
| A     | 73  | ARG  | HB2  | 1.6281     | 0.02        | 2         |
| A     | 103 | GLU  | HG3  | 2.315      | 0.02        | 2         |
| B     | 85  | ASP  | HA   | 4.662      | 0.02        | 1         |
| A     | 115 | GLU  | N    | 119.665    | 0.05        | 1         |
| B     | 69  | MET  | N    | 121.599    | 0.05        | 1         |
| B     | 76  | GLY  | C    | 174.633    | 0.05        | 1         |
| A     | 87  | GLY  | H    | 8.562      | 0.02        | 1         |
| B     | 101 | VAL  | HB   | 2.2517     | 0.02        | 1         |
| B     | 96  | TYR  | HA   | 4.1779     | 0.02        | 1         |
| A     | 108 | THR  | HA   | 3.8489     | 0.02        | 1         |
| B     | 67  | PHE  | N    | 116.555    | 0.05        | 1         |
| A     | 64  | ASP  | CA   | 57.513     | 0.05        | 1         |
| B     | 72  | GLN  | HG2  | 2.555      | 0.02        | 2         |
| A     | 72  | GLN  | HB2  | 2.1875     | 0.02        | 2         |
| A     | 67  | PHE  | CD2  | 130.7586   | 0.05        | 1         |
| B     | 115 | GLU  | H    | 8.4233     | 0.02        | 1         |
| B     | 102 | THR  | HG22 | 1.2612     | 0.02        | 1         |
| A     | 67  | PHE  | C    | 177.788    | 0.05        | 1         |
| B     | 85  | ASP  | HB3  | 2.692      | 0.02        | 1         |
| B     | 70  | LEU  | CB   | 40.583     | 0.05        | 1         |
| B     | 65  | GLU  | H    | 7.8689     | 0.02        | 1         |
| B     | 88  | MET  | CB   | 32.3507    | 0.05        | 1         |
| A     | 99  | ARG  | C    | 178.589    | 0.05        | 1         |
| A     | 99  | ARG  | HB3  | 1.699      | 0.02        | 1         |
| B     | 94  | ARG  | N    | 117.978    | 0.05        | 1         |
| B     | 104 | LEU  | CA   | 58.168     | 0.05        | 1         |
| B     | 109 | ALA  | H    | 7.9484     | 0.02        | 1         |
| B     | 111 | LEU  | HD23 | 1.0021     | 0.02        | 1         |
| A     | 101 | VAL  | C    | 177.268    | 0.05        | 1         |
| B     | 67  | PHE  | C    | 177.788    | 0.05        | 1         |
| A     | 102 | THR  | N    | 115.862    | 0.05        | 1         |
| A     | 69  | MET  | HG2  | 2.7392     | 0.02        | 2         |
| A     | 62  | SER  | HA   | 4.3888     | 0.02        | 1         |
| B     | 80  | LEU  | HA   | 4.2365     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 100 | THR  | CB   | 67.898     | 0.05        | 1         |
| A     | 109 | ALA  | HB2  | 1.5713     | 0.02        | 1         |
| B     | 74  | PHE  | C    | 177.153    | 0.05        | 1         |
| B     | 72  | GLN  | CB   | 28.911     | 0.05        | 1         |
| B     | 89  | THR  | HG22 | 1.2918     | 0.02        | 1         |
| B     | 83  | SER  | N    | 115.637    | 0.05        | 1         |
| B     | 98  | LYS  | N    | 118.058    | 0.05        | 1         |
| B     | 67  | PHE  | HE2  | 7.0507     | 0.02        | 1         |
| B     | 95  | ARG  | HA   | 4.0225     | 0.02        | 1         |
| A     | 62  | SER  | H    | 8.4597     | 0.02        | 1         |
| B     | 108 | THR  | H    | 8.4508     | 0.02        | 1         |
| A     | 89  | THR  | HA   | 3.9534     | 0.02        | 1         |
| A     | 99  | ARG  | H    | 7.8187     | 0.02        | 1         |
| A     | 112 | ARG  | HG3  | 1.685      | 0.02        | 2         |
| B     | 86  | ASN  | HA   | 4.6898     | 0.02        | 1         |
| B     | 73  | ARG  | CA   | 58.095     | 0.05        | 1         |
| A     | 66  | LEU  | HG   | 1.54       | 0.02        | 1         |
| A     | 107 | VAL  | HG23 | 1.0954     | 0.02        | 2         |
| B     | 96  | TYR  | HD1  | 7.2139     | 0.02        | 1         |
| A     | 78  | GLU  | N    | 120.359    | 0.05        | 1         |
| A     | 98  | LYS  | N    | 118.058    | 0.05        | 1         |
| B     | 69  | MET  | CB   | 31.708     | 0.05        | 1         |
| A     | 114 | VAL  | N    | 116.318    | 0.05        | 1         |
| B     | 117 | ARG  | HB2  | 1.926      | 0.02        | 2         |
| A     | 114 | VAL  | CA   | 64.696     | 0.05        | 1         |
| B     | 104 | LEU  | C    | 179.991    | 0.05        | 1         |
| B     | 113 | GLU  | N    | 117.678    | 0.05        | 1         |
| A     | 78  | GLU  | HG2  | 2.2413     | 0.02        | 1         |
| B     | 115 | GLU  | CB   | 30.154     | 0.05        | 1         |
| B     | 101 | VAL  | HG13 | 1.1774     | 0.02        | 2         |
| A     | 75  | GLY  | H    | 7.9742     | 0.02        | 1         |
| B     | 77  | GLY  | CA   | 45.312     | 0.05        | 1         |
| A     | 94  | ARG  | HG3  | 1.524      | 0.02        | 1         |
| B     | 97  | LEU  | CB   | 41.354     | 0.05        | 1         |
| A     | 120 | GLU  | HB3  | 1.926      | 0.02        | 2         |
| B     | 74  | PHE  | CA   | 55.606     | 0.05        | 1         |
| B     | 109 | ALA  | HA   | 4.1425     | 0.02        | 1         |
| B     | 104 | LEU  | HB2  | 2.4038     | 0.02        | 2         |
| B     | 102 | THR  | N    | 115.862    | 0.05        | 1         |
| B     | 107 | VAL  | HB   | 2.1032     | 0.02        | 1         |
| A     | 71  | ASP  | CB   | 40.1067    | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 115 | GLU  | CG   | 37.2644    | 0.05        | 1         |
| B     | 116 | HIS  | HB2  | 3.3644     | 0.02        | 2         |
| A     | 76  | GLY  | C    | 174.633    | 0.05        | 1         |
| B     | 61  | ALA  | C    | 178.053    | 0.05        | 1         |
| A     | 96  | TYR  | HE2  | 6.6582     | 0.02        | 1         |
| A     | 115 | GLU  | HA   | 4.122      | 0.02        | 1         |
| B     | 116 | HIS  | H    | 8.065      | 0.02        | 1         |
| A     | 104 | LEU  | HA   | 4.1554     | 0.02        | 1         |
| A     | 114 | VAL  | C    | 178.062    | 0.05        | 1         |
| A     | 110 | ARG  | H    | 7.7794     | 0.02        | 1         |
| B     | 79  | ASP  | CB   | 40.68      | 0.05        | 1         |
| A     | 72  | GLN  | HG2  | 2.555      | 0.02        | 2         |
| B     | 101 | VAL  | HG23 | 0.9529     | 0.02        | 2         |
| B     | 111 | LEU  | CD1  | 26.404     | 0.05        | 1         |
| B     | 107 | VAL  | CA   | 66.377     | 0.05        | 1         |
| B     | 86  | ASN  | HB2  | 2.86       | 0.02        | 1         |
| A     | 74  | PHE  | N    | 115.746    | 0.05        | 1         |
| B     | 110 | ARG  | C    | 178.434    | 0.05        | 1         |
| B     | 70  | LEU  | HD21 | 0.8188     | 0.02        | 2         |
| A     | 107 | VAL  | CG2  | 22.209     | 0.05        | 2         |
| A     | 111 | LEU  | CD1  | 26.404     | 0.05        | 1         |
| B     | 78  | GLU  | C    | 176.451    | 0.05        | 1         |
| A     | 102 | THR  | HG23 | 1.2612     | 0.02        | 1         |
| A     | 78  | GLU  | CA   | 57.064     | 0.05        | 1         |
| B     | 75  | GLY  | HA3  | 4.0355     | 0.02        | 2         |
| B     | 108 | THR  | HA   | 3.8489     | 0.02        | 1         |
| A     | 97  | LEU  | HA   | 4.3064     | 0.02        | 1         |
| A     | 105 | ASP  | HB2  | 2.9189     | 0.02        | 2         |
| B     | 84  | GLY  | N    | 110.24     | 0.05        | 1         |
| A     | 80  | LEU  | HA   | 4.2365     | 0.02        | 1         |
| A     | 93  | LEU  | CD1  | 28.096     | 0.05        | 2         |
| B     | 120 | GLU  | H    | 7.868      | 0.02        | 1         |
| A     | 88  | MET  | HG2  | 2.692      | 0.02        | 2         |
| B     | 88  | MET  | HB2  | 2.2635     | 0.02        | 2         |
| B     | 111 | LEU  | N    | 120.259    | 0.05        | 1         |
| A     | 89  | THR  | CA   | 66.713     | 0.05        | 1         |
| B     | 79  | ASP  | HB3  | 2.594      | 0.02        | 2         |
| B     | 118 | ALA  | HA   | 4.347      | 0.02        | 1         |
| A     | 72  | GLN  | NE2  | 111.83     | 0.05        | 1         |
| B     | 86  | ASN  | CA   | 54.282     | 0.05        | 1         |
| B     | 101 | VAL  | CG2  | 21.824     | 0.05        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 101 | VAL  | N    | 123.121    | 0.05        | 1         |
| A     | 93  | LEU  | N    | 118.034    | 0.05        | 1         |
| B     | 74  | PHE  | HD2  | 7.1489     | 0.02        | 1         |
| A     | 84  | GLY  | HA2  | 3.99       | 0.02        | 1         |
| A     | 106 | SER  | HA   | 4.3589     | 0.02        | 1         |
| A     | 110 | ARG  | CB   | 29.828     | 0.05        | 1         |
| A     | 107 | VAL  | HB   | 2.1032     | 0.02        | 1         |
| B     | 70  | LEU  | HD11 | 0.9524     | 0.02        | 2         |
| A     | 109 | ALA  | CA   | 55.2767    | 0.05        | 1         |
| B     | 95  | ARG  | HG3  | 1.582      | 0.02        | 2         |
| A     | 101 | VAL  | HG23 | 0.9529     | 0.02        | 2         |
| B     | 70  | LEU  | N    | 121.809    | 0.05        | 1         |
| B     | 65  | GLU  | CG   | 36.6105    | 0.05        | 1         |
| B     | 77  | GLY  | HA2  | 4.0045     | 0.02        | 1         |
| A     | 114 | VAL  | CG1  | 21.731     | 0.05        | 2         |
| A     | 100 | THR  | N    | 118.134    | 0.05        | 1         |
| B     | 111 | LEU  | HB2  | 2.141      | 0.02        | 2         |
| A     | 108 | THR  | H    | 8.4508     | 0.02        | 1         |
| B     | 72  | GLN  | N    | 117.125    | 0.05        | 1         |
| A     | 108 | THR  | HG22 | 1.3239     | 0.02        | 1         |
| B     | 113 | GLU  | HB3  | 2.247      | 0.02        | 1         |
| A     | 118 | ALA  | HB3  | 1.454      | 0.02        | 1         |
| A     | 78  | GLU  | HB3  | 1.9387     | 0.02        | 2         |
| A     | 66  | LEU  | CB   | 41.718     | 0.05        | 1         |
| B     | 87  | GLY  | C    | 177.446    | 0.05        | 1         |
| B     | 80  | LEU  | H    | 8.0598     | 0.02        | 1         |
| A     | 101 | VAL  | CG1  | 24.748     | 0.05        | 2         |
| A     | 92  | LYS  | CB   | 33.037     | 0.05        | 1         |
| B     | 110 | ARG  | H    | 7.7794     | 0.02        | 1         |
| A     | 73  | ARG  | HA   | 4.0762     | 0.02        | 1         |
| A     | 85  | ASP  | N    | 119.831    | 0.05        | 1         |
| B     | 114 | VAL  | HG12 | 1.0836     | 0.02        | 2         |
| A     | 104 | LEU  | CD2  | 23.058     | 0.05        | 2         |
| A     | 94  | ARG  | N    | 117.978    | 0.05        | 1         |
| B     | 78  | GLU  | HB3  | 1.9387     | 0.02        | 2         |
| A     | 111 | LEU  | HD12 | 1.0021     | 0.02        | 1         |
| A     | 110 | ARG  | HB2  | 2.0495     | 0.02        | 1         |
| A     | 108 | THR  | HG23 | 1.3239     | 0.02        | 1         |
| B     | 80  | LEU  | HB2  | 1.553      | 0.02        | 2         |
| A     | 111 | LEU  | HD23 | 1.0021     | 0.02        | 1         |
| B     | 114 | VAL  | CG2  | 21.77      | 0.05        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 67  | PHE  | CA   | 58.826     | 0.05        | 1         |
| B     | 111 | LEU  | CA   | 58.751     | 0.05        | 1         |
| B     | 101 | VAL  | CA   | 67.467     | 0.05        | 1         |
| A     | 67  | PHE  | CD1  | 130.7586   | 0.05        | 1         |
| B     | 116 | HIS  | CA   | 56.424     | 0.05        | 1         |
| A     | 84  | GLY  | C    | 173.946    | 0.05        | 1         |
| A     | 74  | PHE  | HB2  | 3.4556     | 0.02        | 2         |
| A     | 94  | ARG  | HA   | 3.828      | 0.02        | 1         |
| A     | 75  | GLY  | HA3  | 4.0355     | 0.02        | 2         |
| B     | 64  | ASP  | CB   | 40.3157    | 0.05        | 1         |
| A     | 103 | GLU  | H    | 7.8134     | 0.02        | 1         |
| A     | 63  | ASP  | HB2  | 2.4453     | 0.02        | 2         |
| A     | 96  | TYR  | HD1  | 7.2139     | 0.02        | 1         |
| B     | 71  | ASP  | C    | 179.685    | 0.05        | 1         |
| B     | 102 | THR  | CB   | 68.584     | 0.05        | 1         |
| A     | 104 | LEU  | HB3  | 1.4968     | 0.02        | 2         |
| B     | 119 | GLY  | HA3  | 3.9922     | 0.02        | 1         |
| A     | 63  | ASP  | C    | 176.199    | 0.05        | 1         |
| A     | 115 | GLU  | HB2  | 1.985      | 0.02        | 1         |
| A     | 93  | LEU  | HB3  | 1.3173     | 0.02        | 2         |
| A     | 102 | THR  | HA   | 4.041      | 0.02        | 1         |
| B     | 119 | GLY  | CA   | 45.484     | 0.05        | 1         |
| B     | 109 | ALA  | CB   | 17.809     | 0.05        | 1         |
| A     | 112 | ARG  | HD3  | 3.2367     | 0.02        | 1         |
| A     | 97  | LEU  | HB2  | 2.2631     | 0.02        | 1         |
| B     | 84  | GLY  | H    | 8.436      | 0.02        | 1         |
| A     | 66  | LEU  | H    | 7.7568     | 0.02        | 1         |
| B     | 109 | ALA  | HB2  | 1.5713     | 0.02        | 1         |
| B     | 96  | TYR  | N    | 118.48     | 0.05        | 1         |
| B     | 74  | PHE  | HB3  | 3.1222     | 0.02        | 2         |
| B     | 114 | VAL  | HG21 | 0.9746     | 0.02        | 2         |
| B     | 120 | GLU  | HB3  | 1.926      | 0.02        | 2         |
| B     | 73  | ARG  | HG3  | 1.809      | 0.02        | 1         |
| A     | 70  | LEU  | HB3  | 1.3628     | 0.02        | 2         |
| A     | 109 | ALA  | HB1  | 1.5713     | 0.02        | 1         |
| A     | 110 | ARG  | HD3  | 3.2473     | 0.02        | 1         |
| A     | 69  | MET  | H    | 7.926      | 0.02        | 1         |
| B     | 72  | GLN  | CA   | 58.266     | 0.05        | 1         |
| A     | 72  | GLN  | HE22 | 6.85       | 0.02        | 2         |
| B     | 111 | LEU  | C    | 177.945    | 0.05        | 1         |
| A     | 113 | GLU  | HG2  | 2.5467     | 0.02        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 74  | PHE  | CZ   | 130.6045   | 0.05        | 1         |
| A     | 98  | LYS  | C    | 179.251    | 0.05        | 1         |
| A     | 109 | ALA  | HA   | 4.1425     | 0.02        | 1         |
| B     | 93  | LEU  | HD13 | 1.0569     | 0.02        | 2         |
| A     | 95  | ARG  | C    | 180.478    | 0.05        | 1         |
| B     | 111 | LEU  | HD21 | 1.0021     | 0.02        | 1         |
| A     | 65  | GLU  | H    | 7.8689     | 0.02        | 1         |
| B     | 65  | GLU  | C    | 178.519    | 0.05        | 1         |
| A     | 88  | MET  | CA   | 55.345     | 0.05        | 1         |
| B     | 83  | SER  | HB2  | 3.92       | 0.02        | 1         |
| A     | 71  | ASP  | HB2  | 2.945      | 0.02        | 2         |
| B     | 107 | VAL  | H    | 8.7596     | 0.02        | 1         |
| B     | 115 | GLU  | HB3  | 1.985      | 0.02        | 1         |
| B     | 73  | ARG  | H    | 7.776      | 0.02        | 1         |
| B     | 107 | VAL  | HG12 | 1.2189     | 0.02        | 2         |
| A     | 61  | ALA  | CB   | 19.203     | 0.05        | 1         |
| B     | 67  | PHE  | CE1  | 130.187    | 0.05        | 1         |
| B     | 71  | ASP  | N    | 120.316    | 0.05        | 1         |
| A     | 87  | GLY  | HA2  | 4.0        | 0.02        | 1         |
| A     | 97  | LEU  | HB3  | 1.6333     | 0.02        | 1         |
| B     | 79  | ASP  | HA   | 4.5162     | 0.02        | 1         |
| A     | 107 | VAL  | CB   | 31.72      | 0.05        | 1         |
| A     | 95  | ARG  | N    | 118.625    | 0.05        | 1         |
| A     | 78  | GLU  | HB2  | 2.059      | 0.02        | 2         |
| B     | 96  | TYR  | CA   | 63.042     | 0.05        | 1         |
| B     | 64  | ASP  | HA   | 4.3513     | 0.02        | 1         |
| A     | 110 | ARG  | N    | 119.071    | 0.05        | 1         |
| B     | 85  | ASP  | C    | 176.308    | 0.05        | 1         |
| B     | 97  | LEU  | C    | 177.683    | 0.05        | 1         |
| B     | 90  | GLU  | N    | 120.081    | 0.05        | 1         |
| B     | 110 | ARG  | N    | 119.071    | 0.05        | 1         |
| B     | 81  | LEU  | H    | 8.0625     | 0.02        | 1         |
| B     | 99  | ARG  | N    | 117.877    | 0.05        | 1         |
| B     | 95  | ARG  | HB2  | 1.855      | 0.02        | 1         |
| A     | 100 | THR  | HG21 | 1.3291     | 0.02        | 1         |
| B     | 74  | PHE  | CD1  | 131.005    | 0.05        | 1         |
| A     | 105 | ASP  | N    | 123.415    | 0.05        | 1         |
| A     | 96  | TYR  | HE1  | 6.6582     | 0.02        | 1         |
| B     | 93  | LEU  | CD1  | 28.096     | 0.05        | 2         |
| A     | 110 | ARG  | HG3  | 1.483      | 0.02        | 1         |
| A     | 67  | PHE  | H    | 8.455      | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 103 | GLU  | HB3  | 2.024      | 0.02        | 1         |
| B     | 80  | LEU  | C    | 177.403    | 0.05        | 1         |
| A     | 65  | GLU  | HB3  | 2.0165     | 0.02        | 2         |
| B     | 67  | PHE  | HZ   | 6.9597     | 0.02        | 1         |
| A     | 77  | GLY  | CA   | 45.312     | 0.05        | 1         |
| B     | 93  | LEU  | HG   | 2.0344     | 0.02        | 1         |
| A     | 81  | LEU  | HA   | 4.2574     | 0.02        | 1         |
| A     | 73  | ARG  | HG3  | 1.809      | 0.02        | 1         |
| A     | 85  | ASP  | CB   | 41.217     | 0.05        | 1         |
| A     | 67  | PHE  | CE1  | 130.187    | 0.05        | 1         |
| B     | 93  | LEU  | N    | 118.034    | 0.05        | 1         |
| A     | 81  | LEU  | HB3  | 1.5887     | 0.02        | 2         |
| A     | 113 | GLU  | CA   | 58.842     | 0.05        | 1         |
| B     | 110 | ARG  | HB3  | 2.0495     | 0.02        | 1         |
| B     | 88  | MET  | CA   | 55.345     | 0.05        | 1         |
| B     | 94  | ARG  | HG3  | 1.524      | 0.02        | 1         |
| A     | 62  | SER  | CA   | 58.466     | 0.05        | 1         |
| A     | 88  | MET  | N    | 119.486    | 0.05        | 1         |
| A     | 119 | GLY  | N    | 127.342    | 0.05        | 1         |
| A     | 97  | LEU  | CA   | 59.0       | 0.05        | 1         |
| B     | 65  | GLU  | HG3  | 2.22       | 0.02        | 2         |
| A     | 70  | LEU  | HD22 | 0.8188     | 0.02        | 2         |
| A     | 97  | LEU  | HD11 | 1.0221     | 0.02        | 1         |
| B     | 80  | LEU  | N    | 121.42     | 0.05        | 1         |
| A     | 68  | SER  | HA   | 4.3372     | 0.02        | 1         |
| B     | 81  | LEU  | HA   | 4.2574     | 0.02        | 1         |
| A     | 115 | GLU  | CG   | 37.2644    | 0.05        | 1         |
| B     | 69  | MET  | CG   | 31.678     | 0.05        | 1         |
| A     | 72  | GLN  | N    | 117.125    | 0.05        | 1         |
| A     | 85  | ASP  | HA   | 4.662      | 0.02        | 1         |
| B     | 112 | ARG  | CA   | 59.108     | 0.05        | 1         |
| B     | 107 | VAL  | HG21 | 1.0954     | 0.02        | 2         |
| A     | 104 | LEU  | HD13 | 1.1055     | 0.02        | 2         |
| A     | 86  | ASN  | HD21 | 7.648      | 0.02        | 1         |
| A     | 104 | LEU  | HD22 | 0.9838     | 0.02        | 2         |
| B     | 93  | LEU  | HD21 | 0.93       | 0.02        | 2         |
| B     | 112 | ARG  | HD2  | 3.2367     | 0.02        | 1         |
| A     | 89  | THR  | HG23 | 1.2918     | 0.02        | 1         |
| A     | 110 | ARG  | CA   | 58.628     | 0.05        | 1         |
| B     | 96  | TYR  | HB2  | 3.2251     | 0.02        | 2         |
| A     | 104 | LEU  | CA   | 58.168     | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 97  | LEU  | HD23 | 1.0221     | 0.02        | 1         |
| A     | 107 | VAL  | HA   | 3.8852     | 0.02        | 1         |
| A     | 108 | THR  | N    | 116.699    | 0.05        | 1         |
| B     | 103 | GLU  | CA   | 58.964     | 0.05        | 1         |
| A     | 72  | GLN  | H    | 7.6168     | 0.02        | 1         |
| A     | 65  | GLU  | C    | 178.519    | 0.05        | 1         |
| A     | 68  | SER  | CA   | 61.769     | 0.05        | 1         |
| A     | 114 | VAL  | CG2  | 21.77      | 0.05        | 2         |
| B     | 87  | GLY  | N    | 127.57     | 0.05        | 1         |
| B     | 94  | ARG  | C    | 178.078    | 0.05        | 1         |
| B     | 106 | SER  | CB   | 62.755     | 0.05        | 1         |
| B     | 108 | THR  | HG21 | 1.3239     | 0.02        | 1         |
| A     | 77  | GLY  | N    | 127.741    | 0.05        | 1         |
| B     | 97  | LEU  | H    | 9.2677     | 0.02        | 1         |
| B     | 70  | LEU  | HB2  | 2.021      | 0.02        | 2         |
| A     | 80  | LEU  | CB   | 41.854     | 0.05        | 1         |
| B     | 66  | LEU  | C    | 178.453    | 0.05        | 1         |
| B     | 69  | MET  | HA   | 4.1346     | 0.02        | 1         |
| A     | 113 | GLU  | N    | 117.678    | 0.05        | 1         |
| B     | 117 | ARG  | CA   | 56.541     | 0.05        | 1         |
| B     | 106 | SER  | HA   | 4.3589     | 0.02        | 1         |
| A     | 67  | PHE  | HE2  | 7.0507     | 0.02        | 1         |
| B     | 96  | TYR  | HE1  | 6.6582     | 0.02        | 1         |
| A     | 97  | LEU  | N    | 124.775    | 0.05        | 1         |
| B     | 104 | LEU  | HD23 | 0.9838     | 0.02        | 2         |
| B     | 72  | GLN  | HB2  | 2.1875     | 0.02        | 2         |
| B     | 110 | ARG  | HG2  | 1.483      | 0.02        | 1         |
| A     | 70  | LEU  | HD12 | 0.9524     | 0.02        | 2         |
| A     | 81  | LEU  | N    | 120.607    | 0.05        | 1         |
| A     | 90  | GLU  | CA   | 60.941     | 0.05        | 1         |
| B     | 97  | LEU  | HD12 | 1.0221     | 0.02        | 1         |
| A     | 68  | SER  | C    | 177.344    | 0.05        | 1         |
| A     | 111 | LEU  | N    | 120.259    | 0.05        | 1         |
| B     | 105 | ASP  | C    | 179.011    | 0.05        | 1         |
| A     | 78  | GLU  | CB   | 30.027     | 0.05        | 1         |
| B     | 71  | ASP  | CB   | 40.1067    | 0.05        | 1         |
| B     | 64  | ASP  | CA   | 57.513     | 0.05        | 1         |
| A     | 96  | TYR  | HD2  | 7.2139     | 0.02        | 1         |
| B     | 114 | VAL  | H    | 8.033      | 0.02        | 1         |
| A     | 93  | LEU  | HD23 | 0.93       | 0.02        | 2         |
| B     | 111 | LEU  | HD11 | 1.0021     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 97  | LEU  | CD2  | 27.251     | 0.05        | 1         |
| A     | 104 | LEU  | N    | 121.08     | 0.05        | 1         |
| B     | 76  | GLY  | HA2  | 4.129      | 0.02        | 2         |
| A     | 87  | GLY  | CA   | 45.746     | 0.05        | 1         |
| A     | 118 | ALA  | N    | 123.787    | 0.05        | 1         |
| A     | 71  | ASP  | HA   | 4.4852     | 0.02        | 1         |
| A     | 110 | ARG  | C    | 178.434    | 0.05        | 1         |
| A     | 105 | ASP  | CB   | 39.5007    | 0.05        | 1         |
| A     | 80  | LEU  | H    | 8.0598     | 0.02        | 1         |
| B     | 97  | LEU  | HD21 | 1.0221     | 0.02        | 1         |
| A     | 117 | ARG  | HB3  | 1.8478     | 0.02        | 2         |
| B     | 84  | GLY  | HA2  | 3.99       | 0.02        | 1         |
| B     | 96  | TYR  | CD2  | 132.505    | 0.05        | 1         |
| A     | 86  | ASN  | HA   | 4.6898     | 0.02        | 1         |
| B     | 101 | VAL  | N    | 123.121    | 0.05        | 1         |
| B     | 100 | THR  | HG22 | 1.3291     | 0.02        | 1         |
| A     | 112 | ARG  | C    | 178.907    | 0.05        | 1         |
| A     | 115 | GLU  | H    | 8.4233     | 0.02        | 1         |
| A     | 116 | HIS  | CD2  | 120.098    | 0.05        | 1         |
| B     | 67  | PHE  | H    | 8.455      | 0.02        | 1         |
| A     | 70  | LEU  | H    | 8.3178     | 0.02        | 1         |
| A     | 98  | LYS  | HB3  | 1.8925     | 0.02        | 1         |
| A     | 61  | ALA  | HB1  | 1.3784     | 0.02        | 1         |
| B     | 67  | PHE  | CD2  | 130.7586   | 0.05        | 1         |
| B     | 71  | ASP  | H    | 8.9831     | 0.02        | 1         |
| A     | 76  | GLY  | HA2  | 4.129      | 0.02        | 2         |
| A     | 119 | GLY  | HA2  | 3.9922     | 0.02        | 1         |
| B     | 73  | ARG  | HB2  | 1.6281     | 0.02        | 2         |
| B     | 104 | LEU  | CD1  | 26.18      | 0.05        | 2         |
| A     | 66  | LEU  | HB3  | 1.521      | 0.02        | 1         |
| A     | 73  | ARG  | HB3  | 1.4748     | 0.02        | 2         |
| A     | 61  | ALA  | CA   | 52.678     | 0.05        | 1         |
| A     | 73  | ARG  | C    | 178.187    | 0.05        | 1         |
| A     | 93  | LEU  | HD11 | 1.0569     | 0.02        | 2         |
| A     | 100 | THR  | CG2  | 22.547     | 0.05        | 1         |
| B     | 94  | ARG  | H    | 8.3326     | 0.02        | 1         |
| B     | 100 | THR  | N    | 118.134    | 0.05        | 1         |
| A     | 110 | ARG  | HA   | 4.16       | 0.02        | 1         |
| A     | 93  | LEU  | CG   | 27.448     | 0.05        | 1         |
| A     | 117 | ARG  | H    | 8.101      | 0.02        | 1         |
| A     | 69  | MET  | HB2  | 2.2694     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 71  | ASP  | N    | 120.316    | 0.05        | 1         |
| B     | 91  | GLU  | H    | 7.618      | 0.02        | 1         |
| B     | 83  | SER  | H    | 8.231      | 0.02        | 1         |
| A     | 79  | ASP  | H    | 8.5087     | 0.02        | 1         |
| B     | 108 | THR  | N    | 116.699    | 0.05        | 1         |
| A     | 118 | ALA  | CA   | 52.761     | 0.05        | 1         |
| A     | 100 | THR  | HG22 | 1.3291     | 0.02        | 1         |
| A     | 67  | PHE  | HZ   | 6.9597     | 0.02        | 1         |
| A     | 102 | THR  | HG21 | 1.2612     | 0.02        | 1         |
| A     | 111 | LEU  | HA   | 4.1023     | 0.02        | 1         |
| B     | 69  | MET  | CA   | 59.008     | 0.05        | 1         |
| B     | 115 | GLU  | C    | 177.308    | 0.05        | 1         |
| A     | 69  | MET  | HG3  | 2.5146     | 0.02        | 2         |
| B     | 63  | ASP  | H    | 8.5392     | 0.02        | 1         |
| A     | 72  | GLN  | HE21 | 7.434      | 0.02        | 2         |
| B     | 70  | LEU  | CD2  | 21.72      | 0.05        | 2         |
| A     | 66  | LEU  | C    | 178.453    | 0.05        | 1         |
| B     | 106 | SER  | HB2  | 4.0969     | 0.02        | 2         |
| A     | 100 | THR  | C    | 176.489    | 0.05        | 1         |
| A     | 92  | LYS  | HA   | 3.9304     | 0.02        | 1         |
| B     | 86  | ASN  | CB   | 38.802     | 0.05        | 1         |
| A     | 73  | ARG  | CA   | 58.095     | 0.05        | 1         |
| A     | 120 | GLU  | HA   | 4.171      | 0.02        | 1         |
| B     | 62  | SER  | HB2  | 4.087      | 0.02        | 2         |
| B     | 112 | ARG  | HG3  | 1.685      | 0.02        | 2         |
| A     | 89  | THR  | HB   | 4.222      | 0.02        | 1         |
| A     | 76  | GLY  | H    | 8.4573     | 0.02        | 1         |
| A     | 68  | SER  | H    | 8.0576     | 0.02        | 1         |
| A     | 80  | LEU  | N    | 121.42     | 0.05        | 1         |
| A     | 67  | PHE  | CE2  | 130.187    | 0.05        | 1         |
| A     | 117 | ARG  | HD3  | 3.244      | 0.02        | 1         |
| A     | 70  | LEU  | CD1  | 26.747     | 0.05        | 2         |
| B     | 102 | THR  | HG21 | 1.2612     | 0.02        | 1         |
| A     | 112 | ARG  | CD   | 43.449     | 0.05        | 1         |
| B     | 88  | MET  | HA   | 4.6645     | 0.02        | 1         |
| B     | 110 | ARG  | CA   | 58.628     | 0.05        | 1         |
| A     | 106 | SER  | N    | 117.055    | 0.05        | 1         |
| A     | 102 | THR  | HB   | 4.2957     | 0.02        | 1         |
| A     | 78  | GLU  | HG3  | 2.2413     | 0.02        | 1         |
| B     | 97  | LEU  | CD1  | 27.251     | 0.05        | 1         |
| B     | 81  | LEU  | N    | 120.607    | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 114 | VAL  | HA   | 3.9892     | 0.02        | 1         |
| B     | 115 | GLU  | CA   | 58.678     | 0.05        | 1         |
| A     | 111 | LEU  | CB   | 41.5949    | 0.05        | 1         |
| A     | 102 | THR  | C    | 177.031    | 0.05        | 1         |
| A     | 106 | SER  | HB2  | 4.0969     | 0.02        | 2         |
| B     | 85  | ASP  | H    | 8.212      | 0.02        | 1         |
| A     | 117 | ARG  | HG2  | 1.72       | 0.02        | 1         |
| A     | 97  | LEU  | H    | 9.2677     | 0.02        | 1         |
| B     | 62  | SER  | N    | 116.091    | 0.05        | 1         |
| A     | 71  | ASP  | C    | 179.685    | 0.05        | 1         |
| B     | 98  | LYS  | C    | 179.251    | 0.05        | 1         |
| B     | 116 | HIS  | HB3  | 3.2742     | 0.02        | 2         |
| B     | 107 | VAL  | CG1  | 22.534     | 0.05        | 2         |
| B     | 101 | VAL  | C    | 177.268    | 0.05        | 1         |
| A     | 77  | GLY  | H    | 8.415      | 0.02        | 1         |
| A     | 106 | SER  | H    | 8.1317     | 0.02        | 1         |
| A     | 90  | GLU  | HA   | 3.8232     | 0.02        | 1         |
| B     | 119 | GLY  | N    | 127.342    | 0.05        | 1         |
| A     | 101 | VAL  | HG22 | 0.9529     | 0.02        | 2         |
| A     | 68  | SER  | CB   | 62.758     | 0.05        | 1         |
| B     | 118 | ALA  | HB3  | 1.454      | 0.02        | 1         |
| A     | 64  | ASP  | HB2  | 2.668      | 0.02        | 2         |
| A     | 105 | ASP  | C    | 179.011    | 0.05        | 1         |
| B     | 79  | ASP  | CA   | 54.726     | 0.05        | 1         |
| B     | 116 | HIS  | CD2  | 120.098    | 0.05        | 1         |
| B     | 101 | VAL  | HG22 | 0.9529     | 0.02        | 2         |
| A     | 63  | ASP  | HB3  | 2.2455     | 0.02        | 2         |
| B     | 78  | GLU  | HG3  | 2.2413     | 0.02        | 1         |
| B     | 111 | LEU  | CD2  | 26.404     | 0.05        | 1         |
| B     | 104 | LEU  | H    | 8.9435     | 0.02        | 1         |
| A     | 73  | ARG  | N    | 119.296    | 0.05        | 1         |
| A     | 96  | TYR  | HB2  | 3.2251     | 0.02        | 2         |
| B     | 61  | ALA  | HB1  | 1.3784     | 0.02        | 1         |
| A     | 82  | MET  | HB2  | 2.111      | 0.02        | 2         |
| B     | 96  | TYR  | H    | 8.8287     | 0.02        | 1         |
| B     | 70  | LEU  | HA   | 3.7548     | 0.02        | 1         |
| B     | 101 | VAL  | CB   | 31.411     | 0.05        | 1         |
| B     | 90  | GLU  | H    | 9.0826     | 0.02        | 1         |
| A     | 74  | PHE  | HE2  | 7.3494     | 0.02        | 1         |
| B     | 116 | HIS  | HD2  | 7.2787     | 0.02        | 1         |
| B     | 83  | SER  | HA   | 4.4163     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 72  | GLN  | HG3  | 2.416      | 0.02        | 2         |
| A     | 103 | GLU  | C    | 178.219    | 0.05        | 1         |
| A     | 111 | LEU  | H    | 8.4697     | 0.02        | 1         |
| A     | 104 | LEU  | CG   | 27.402     | 0.05        | 1         |
| A     | 97  | LEU  | HD21 | 1.0221     | 0.02        | 1         |
| A     | 61  | ALA  | H    | 8.278      | 0.02        | 1         |
| A     | 83  | SER  | N    | 115.637    | 0.05        | 1         |
| B     | 82  | MET  | HB3  | 2.027      | 0.02        | 2         |
| A     | 70  | LEU  | HD11 | 0.9524     | 0.02        | 2         |
| B     | 99  | ARG  | HA   | 4.1907     | 0.02        | 1         |
| A     | 74  | PHE  | HZ   | 7.19       | 0.02        | 1         |
| B     | 97  | LEU  | HD11 | 1.0221     | 0.02        | 1         |
| B     | 79  | ASP  | HB2  | 2.7017     | 0.02        | 2         |
| B     | 103 | GLU  | H    | 7.8134     | 0.02        | 1         |
| B     | 70  | LEU  | C    | 178.045    | 0.05        | 1         |
| A     | 108 | THR  | CB   | 68.701     | 0.05        | 1         |
| B     | 104 | LEU  | HD13 | 1.1055     | 0.02        | 2         |
| B     | 70  | LEU  | HD12 | 0.9524     | 0.02        | 2         |
| B     | 74  | PHE  | HD1  | 7.1489     | 0.02        | 1         |
| B     | 118 | ALA  | HB1  | 1.454      | 0.02        | 1         |
| B     | 90  | GLU  | C    | 176.85     | 0.05        | 1         |
| B     | 98  | LYS  | HB2  | 1.8925     | 0.02        | 1         |
| B     | 77  | GLY  | C    | 174.525    | 0.05        | 1         |
| B     | 66  | LEU  | H    | 7.7568     | 0.02        | 1         |
| B     | 94  | ARG  | HA   | 3.828      | 0.02        | 1         |
| A     | 61  | ALA  | HA   | 4.336      | 0.02        | 1         |
| B     | 117 | ARG  | HD3  | 3.244      | 0.02        | 1         |
| A     | 70  | LEU  | HG   | 1.96       | 0.02        | 1         |
| A     | 97  | LEU  | CD1  | 27.251     | 0.05        | 1         |
| B     | 77  | GLY  | HA3  | 4.0045     | 0.02        | 1         |
| A     | 108 | THR  | HG21 | 1.3239     | 0.02        | 1         |
| A     | 101 | VAL  | H    | 8.6682     | 0.02        | 1         |
| B     | 76  | GLY  | H    | 8.4573     | 0.02        | 1         |
| B     | 112 | ARG  | HB2  | 1.9968     | 0.02        | 1         |
| B     | 85  | ASP  | N    | 119.831    | 0.05        | 1         |
| A     | 118 | ALA  | HB2  | 1.454      | 0.02        | 1         |
| B     | 99  | ARG  | H    | 7.8187     | 0.02        | 1         |
| A     | 72  | GLN  | CA   | 58.266     | 0.05        | 1         |
| A     | 113 | GLU  | HA   | 4.1707     | 0.02        | 1         |
| B     | 67  | PHE  | HA   | 4.1112     | 0.02        | 1         |
| A     | 101 | VAL  | CG2  | 21.824     | 0.05        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 96  | TYR  | CA   | 63.042     | 0.05        | 1         |
| A     | 92  | LYS  | CA   | 60.59      | 0.05        | 1         |
| B     | 72  | GLN  | C    | 178.127    | 0.05        | 1         |
| B     | 89  | THR  | CG2  | 22.326     | 0.05        | 1         |
| B     | 105 | ASP  | HA   | 4.5076     | 0.02        | 1         |
| A     | 112 | ARG  | HD2  | 3.2367     | 0.02        | 1         |
| A     | 104 | LEU  | CD1  | 26.18      | 0.05        | 2         |
| A     | 98  | LYS  | CA   | 60.696     | 0.05        | 1         |
| A     | 112 | ARG  | HA   | 4.1704     | 0.02        | 1         |
| A     | 111 | LEU  | HD22 | 1.0021     | 0.02        | 1         |
| B     | 114 | VAL  | CG1  | 21.731     | 0.05        | 2         |
| B     | 65  | GLU  | HA   | 4.0222     | 0.02        | 1         |
| B     | 68  | SER  | N    | 132.064    | 0.05        | 1         |
| B     | 119 | GLY  | C    | 173.361    | 0.05        | 1         |
| B     | 66  | LEU  | CB   | 41.718     | 0.05        | 1         |
| B     | 64  | ASP  | HB2  | 2.668      | 0.02        | 2         |
| A     | 119 | GLY  | H    | 8.2435     | 0.02        | 1         |
| B     | 117 | ARG  | C    | 176.277    | 0.05        | 1         |
| B     | 74  | PHE  | CZ   | 130.6045   | 0.05        | 1         |
| B     | 81  | LEU  | CA   | 55.67      | 0.05        | 1         |
| A     | 75  | GLY  | HA2  | 4.254      | 0.02        | 2         |
| A     | 86  | ASN  | CA   | 54.282     | 0.05        | 1         |
| A     | 116 | HIS  | HE1  | 8.422      | 0.02        | 1         |
| B     | 87  | GLY  | HA3  | 4.0        | 0.02        | 1         |
| A     | 83  | SER  | H    | 8.231      | 0.02        | 1         |
| B     | 102 | THR  | CA   | 66.896     | 0.05        | 1         |
| A     | 90  | GLU  | H    | 9.0826     | 0.02        | 1         |
| B     | 109 | ALA  | C    | 180.452    | 0.05        | 1         |
| A     | 96  | TYR  | C    | 179.519    | 0.05        | 1         |
| A     | 89  | THR  | H    | 8.3848     | 0.02        | 1         |
| A     | 115 | GLU  | HB3  | 1.985      | 0.02        | 1         |
| A     | 101 | VAL  | HG13 | 1.1774     | 0.02        | 2         |
| A     | 63  | ASP  | CB   | 39.686     | 0.05        | 1         |
| A     | 84  | GLY  | CA   | 45.312     | 0.05        | 1         |
| B     | 74  | PHE  | HB2  | 3.4556     | 0.02        | 2         |
| B     | 80  | LEU  | HG   | 1.562      | 0.02        | 1         |
| B     | 117 | ARG  | HG2  | 1.72       | 0.02        | 1         |
| A     | 70  | LEU  | HB2  | 2.021      | 0.02        | 2         |
| A     | 67  | PHE  | HD1  | 6.6752     | 0.02        | 1         |
| A     | 110 | ARG  | HD2  | 3.2473     | 0.02        | 1         |
| B     | 100 | THR  | HA   | 4.3533     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 83  | SER  | HB3  | 3.92       | 0.02        | 1         |
| B     | 74  | PHE  | HE1  | 7.3494     | 0.02        | 1         |
| A     | 96  | TYR  | N    | 118.48     | 0.05        | 1         |
| B     | 118 | ALA  | CA   | 52.761     | 0.05        | 1         |
| A     | 86  | ASN  | C    | 175.824    | 0.05        | 1         |
| B     | 100 | THR  | CG2  | 22.547     | 0.05        | 1         |
| A     | 114 | VAL  | HG12 | 1.0836     | 0.02        | 2         |
| B     | 93  | LEU  | HB3  | 1.3173     | 0.02        | 2         |
| B     | 93  | LEU  | HD12 | 1.0569     | 0.02        | 2         |
| B     | 114 | VAL  | HG11 | 1.0836     | 0.02        | 2         |
| B     | 66  | LEU  | HB3  | 1.521      | 0.02        | 1         |
| A     | 79  | ASP  | CA   | 54.726     | 0.05        | 1         |
| B     | 72  | GLN  | HA   | 4.0676     | 0.02        | 1         |
| B     | 93  | LEU  | CB   | 44.045     | 0.05        | 1         |
| B     | 102 | THR  | C    | 177.031    | 0.05        | 1         |
| A     | 112 | ARG  | CG   | 27.5807    | 0.05        | 1         |
| A     | 117 | ARG  | HB2  | 1.926      | 0.02        | 2         |
| A     | 88  | MET  | CB   | 32.3507    | 0.05        | 1         |
| B     | 89  | THR  | HG21 | 1.2918     | 0.02        | 1         |
| B     | 83  | SER  | HB3  | 3.92       | 0.02        | 1         |
| A     | 64  | ASP  | HA   | 4.3513     | 0.02        | 1         |
| B     | 69  | MET  | C    | 179.38     | 0.05        | 1         |
| A     | 71  | ASP  | HB3  | 2.6608     | 0.02        | 2         |
| B     | 88  | MET  | C    | 176.89     | 0.05        | 1         |
| B     | 80  | LEU  | CB   | 41.854     | 0.05        | 1         |
| B     | 89  | THR  | CA   | 66.713     | 0.05        | 1         |
| B     | 91  | GLU  | C    | 178.68     | 0.05        | 1         |
| B     | 84  | GLY  | CA   | 45.312     | 0.05        | 1         |
| B     | 101 | VAL  | HG11 | 1.1774     | 0.02        | 2         |
| A     | 72  | GLN  | HA   | 4.0676     | 0.02        | 1         |
| B     | 114 | VAL  | HG13 | 1.0836     | 0.02        | 2         |
| A     | 70  | LEU  | C    | 178.045    | 0.05        | 1         |
| A     | 86  | ASN  | N    | 118.739    | 0.05        | 1         |
| A     | 107 | VAL  | HG13 | 1.2189     | 0.02        | 2         |
| B     | 99  | ARG  | HB3  | 1.699      | 0.02        | 1         |
| A     | 117 | ARG  | CA   | 56.541     | 0.05        | 1         |
| B     | 90  | GLU  | HA   | 3.8232     | 0.02        | 1         |
| B     | 116 | HIS  | N    | 117.217    | 0.05        | 1         |
| B     | 61  | ALA  | CA   | 52.678     | 0.05        | 1         |
| B     | 118 | ALA  | C    | 178.096    | 0.05        | 1         |
| B     | 97  | LEU  | HB2  | 2.2631     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 110 | ARG  | HD2  | 3.2473     | 0.02        | 1         |
| B     | 82  | MET  | C    | 176.221    | 0.05        | 1         |
| B     | 114 | VAL  | N    | 116.318    | 0.05        | 1         |
| B     | 118 | ALA  | N    | 123.787    | 0.05        | 1         |
| B     | 96  | TYR  | CE1  | 118.4737   | 0.05        | 1         |
| B     | 74  | PHE  | CD2  | 131.005    | 0.05        | 1         |
| A     | 104 | LEU  | HG   | 1.6745     | 0.02        | 1         |
| B     | 90  | GLU  | CG   | 37.062     | 0.05        | 1         |
| A     | 93  | LEU  | HG   | 2.0344     | 0.02        | 1         |
| B     | 95  | ARG  | N    | 118.625    | 0.05        | 1         |
| B     | 101 | VAL  | HG21 | 0.9529     | 0.02        | 2         |
| A     | 74  | PHE  | HD1  | 7.1489     | 0.02        | 1         |
| B     | 89  | THR  | C    | 175.73     | 0.05        | 1         |
| A     | 65  | GLU  | HB2  | 2.093      | 0.02        | 2         |
| B     | 112 | ARG  | N    | 116.931    | 0.05        | 1         |
| B     | 61  | ALA  | HB2  | 1.3784     | 0.02        | 1         |
| A     | 97  | LEU  | HG   | 1.639      | 0.02        | 1         |
| A     | 114 | VAL  | HG13 | 1.0836     | 0.02        | 2         |
| B     | 78  | GLU  | CA   | 57.064     | 0.05        | 1         |
| B     | 113 | GLU  | H    | 7.711      | 0.02        | 1         |
| A     | 103 | GLU  | HB3  | 2.024      | 0.02        | 1         |
| A     | 73  | ARG  | HG2  | 1.809      | 0.02        | 1         |
| A     | 74  | PHE  | HE1  | 7.3494     | 0.02        | 1         |
| A     | 81  | LEU  | HB2  | 1.6756     | 0.02        | 2         |
| A     | 113 | GLU  | CB   | 29.797     | 0.05        | 1         |
| B     | 94  | ARG  | HG2  | 1.524      | 0.02        | 1         |
| A     | 62  | SER  | CB   | 63.972     | 0.05        | 1         |
| B     | 115 | GLU  | HG2  | 2.4338     | 0.02        | 2         |
| A     | 97  | LEU  | CB   | 41.354     | 0.05        | 1         |
| A     | 96  | TYR  | H    | 8.8287     | 0.02        | 1         |
| A     | 67  | PHE  | HB2  | 3.1709     | 0.02        | 2         |
| A     | 66  | LEU  | HB2  | 1.521      | 0.02        | 1         |
| A     | 70  | LEU  | HD23 | 0.8188     | 0.02        | 2         |
| A     | 97  | LEU  | HD12 | 1.0221     | 0.02        | 1         |
| A     | 89  | THR  | C    | 175.73     | 0.05        | 1         |
| B     | 106 | SER  | C    | 177.693    | 0.05        | 1         |
| A     | 114 | VAL  | HG22 | 0.9746     | 0.02        | 2         |
| A     | 116 | HIS  | HB3  | 3.2742     | 0.02        | 2         |
| A     | 90  | GLU  | CG   | 37.062     | 0.05        | 1         |
| A     | 69  | MET  | HB3  | 2.2694     | 0.02        | 1         |
| A     | 99  | ARG  | HA   | 4.1907     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 68  | SER  | CB   | 62.758     | 0.05        | 1         |
| A     | 62  | SER  | HB2  | 4.087      | 0.02        | 2         |
| A     | 79  | ASP  | HB2  | 2.7017     | 0.02        | 2         |
| B     | 66  | LEU  | N    | 122.23     | 0.05        | 1         |
| A     | 65  | GLU  | CG   | 36.6105    | 0.05        | 1         |
| A     | 113 | GLU  | HB2  | 2.247      | 0.02        | 1         |
| B     | 104 | LEU  | HG   | 1.6745     | 0.02        | 1         |
| B     | 72  | GLN  | NE2  | 111.83     | 0.05        | 1         |
| B     | 92  | LYS  | HA   | 3.9304     | 0.02        | 1         |
| B     | 112 | ARG  | HD3  | 3.2367     | 0.02        | 1         |
| B     | 90  | GLU  | HB2  | 2.2598     | 0.02        | 2         |
| A     | 89  | THR  | HG22 | 1.2918     | 0.02        | 1         |
| A     | 65  | GLU  | HG2  | 2.308      | 0.02        | 2         |
| B     | 92  | LYS  | CA   | 60.59      | 0.05        | 1         |
| B     | 118 | ALA  | HB2  | 1.454      | 0.02        | 1         |
| B     | 87  | GLY  | H    | 8.562      | 0.02        | 1         |
| A     | 104 | LEU  | CB   | 41.847     | 0.05        | 1         |
| B     | 90  | GLU  | HG3  | 2.1665     | 0.02        | 1         |
| B     | 88  | MET  | N    | 119.486    | 0.05        | 1         |
| A     | 86  | ASN  | H    | 8.507      | 0.02        | 1         |
| A     | 119 | GLY  | CA   | 45.484     | 0.05        | 1         |
| A     | 111 | LEU  | C    | 177.945    | 0.05        | 1         |
| B     | 82  | MET  | HA   | 4.486      | 0.02        | 1         |
| A     | 89  | THR  | CG2  | 22.326     | 0.05        | 1         |
| A     | 88  | MET  | HA   | 4.6645     | 0.02        | 1         |
| B     | 106 | SER  | N    | 117.055    | 0.05        | 1         |
| A     | 71  | ASP  | H    | 8.9831     | 0.02        | 1         |
| B     | 106 | SER  | CA   | 61.691     | 0.05        | 1         |
| B     | 75  | GLY  | N    | 127.302    | 0.05        | 1         |
| A     | 112 | ARG  | HG2  | 1.8422     | 0.02        | 2         |
| A     | 96  | TYR  | CB   | 38.15      | 0.05        | 1         |
| B     | 78  | GLU  | N    | 120.359    | 0.05        | 1         |
| B     | 70  | LEU  | HB3  | 1.3628     | 0.02        | 2         |
| B     | 101 | VAL  | H    | 8.6682     | 0.02        | 1         |
| B     | 79  | ASP  | H    | 8.5087     | 0.02        | 1         |
| B     | 81  | LEU  | HB2  | 1.6756     | 0.02        | 2         |
| A     | 64  | ASP  | CB   | 40.3157    | 0.05        | 1         |
| A     | 72  | GLN  | HB3  | 2.0145     | 0.02        | 2         |
| B     | 105 | ASP  | CB   | 39.5007    | 0.05        | 1         |
| A     | 114 | VAL  | CB   | 32.09      | 0.05        | 1         |
| A     | 114 | VAL  | HB   | 2.2135     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 90  | GLU  | HG2  | 2.1665     | 0.02        | 1         |
| A     | 92  | LYS  | HB3  | 1.709      | 0.02        | 2         |
| B     | 96  | TYR  | HE2  | 6.6582     | 0.02        | 1         |
| B     | 112 | ARG  | H    | 8.1463     | 0.02        | 1         |
| B     | 65  | GLU  | HG2  | 2.308      | 0.02        | 2         |
| A     | 77  | GLY  | C    | 174.525    | 0.05        | 1         |
| B     | 105 | ASP  | CA   | 57.826     | 0.05        | 1         |
| B     | 75  | GLY  | C    | 174.75     | 0.05        | 1         |
| A     | 91  | GLU  | HA   | 4.1593     | 0.02        | 1         |
| A     | 108 | THR  | C    | 176.228    | 0.05        | 1         |
| A     | 63  | ASP  | HA   | 4.0461     | 0.02        | 1         |
| A     | 112 | ARG  | H    | 8.1463     | 0.02        | 1         |
| B     | 66  | LEU  | CA   | 58.092     | 0.05        | 1         |
| B     | 78  | GLU  | HA   | 4.2436     | 0.02        | 1         |
| B     | 97  | LEU  | HA   | 4.3064     | 0.02        | 1         |
| A     | 117 | ARG  | HA   | 4.2938     | 0.02        | 1         |
| B     | 95  | ARG  | C    | 180.478    | 0.05        | 1         |
| B     | 71  | ASP  | CA   | 57.618     | 0.05        | 1         |
| A     | 86  | ASN  | CB   | 38.802     | 0.05        | 1         |
| B     | 61  | ALA  | HA   | 4.336      | 0.02        | 1         |
| A     | 93  | LEU  | HD22 | 0.93       | 0.02        | 2         |
| B     | 82  | MET  | HB2  | 2.111      | 0.02        | 2         |
| B     | 86  | ASN  | ND2  | 112.62     | 0.05        | 1         |
| B     | 100 | THR  | CB   | 67.898     | 0.05        | 1         |
| A     | 117 | ARG  | HG3  | 1.72       | 0.02        | 1         |
| B     | 70  | LEU  | HG   | 1.96       | 0.02        | 1         |
| B     | 74  | PHE  | HA   | 5.0077     | 0.02        | 1         |
| B     | 69  | MET  | H    | 7.926      | 0.02        | 1         |
| A     | 100 | THR  | H    | 8.5228     | 0.02        | 1         |
| B     | 105 | ASP  | HB2  | 2.9189     | 0.02        | 2         |
| B     | 116 | HIS  | CB   | 28.596     | 0.05        | 1         |
| A     | 67  | PHE  | HE1  | 7.0507     | 0.02        | 1         |
| A     | 69  | MET  | CG   | 31.678     | 0.05        | 1         |
| B     | 72  | GLN  | H    | 7.6168     | 0.02        | 1         |
| B     | 108 | THR  | CB   | 68.701     | 0.05        | 1         |
| B     | 88  | MET  | HG2  | 2.692      | 0.02        | 2         |
| A     | 105 | ASP  | CA   | 57.826     | 0.05        | 1         |
| A     | 115 | GLU  | HG3  | 2.1355     | 0.02        | 2         |
| B     | 116 | HIS  | HE1  | 8.422      | 0.02        | 1         |
| B     | 114 | VAL  | HG23 | 0.9746     | 0.02        | 2         |
| A     | 67  | PHE  | HD2  | 6.6752     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 106 | SER  | C    | 177.693    | 0.05        | 1         |
| A     | 64  | ASP  | H    | 8.028      | 0.02        | 1         |
| B     | 84  | GLY  | HA3  | 3.99       | 0.02        | 1         |
| B     | 112 | ARG  | CB   | 30.017     | 0.05        | 1         |
| B     | 112 | ARG  | CG   | 27.5807    | 0.05        | 1         |
| A     | 95  | ARG  | HB2  | 1.855      | 0.02        | 1         |
| B     | 100 | THR  | HG21 | 1.3291     | 0.02        | 1         |
| B     | 93  | LEU  | HD11 | 1.0569     | 0.02        | 2         |
| B     | 111 | LEU  | HG   | 1.717      | 0.02        | 1         |
| B     | 75  | GLY  | CA   | 45.837     | 0.05        | 1         |
| A     | 112 | ARG  | CB   | 30.017     | 0.05        | 1         |
| A     | 112 | ARG  | HB3  | 1.9968     | 0.02        | 1         |
| A     | 88  | MET  | C    | 176.89     | 0.05        | 1         |
| A     | 98  | LYS  | HB2  | 1.8925     | 0.02        | 1         |
| A     | 62  | SER  | N    | 116.091    | 0.05        | 1         |
| A     | 88  | MET  | CG   | 32.3075    | 0.05        | 1         |
| B     | 73  | ARG  | C    | 178.187    | 0.05        | 1         |
| B     | 97  | LEU  | HD22 | 1.0221     | 0.02        | 1         |
| B     | 100 | THR  | H    | 8.5228     | 0.02        | 1         |
| B     | 80  | LEU  | CA   | 55.592     | 0.05        | 1         |
| B     | 92  | LYS  | HB2  | 1.8253     | 0.02        | 2         |
| B     | 112 | ARG  | HG2  | 1.8422     | 0.02        | 2         |
| A     | 93  | LEU  | HD12 | 1.0569     | 0.02        | 2         |
| A     | 104 | LEU  | HD21 | 0.9838     | 0.02        | 2         |
| B     | 113 | GLU  | CA   | 58.842     | 0.05        | 1         |
| B     | 104 | LEU  | HD12 | 1.1055     | 0.02        | 2         |
| B     | 62  | SER  | CB   | 63.972     | 0.05        | 1         |
| A     | 117 | ARG  | CB   | 30.615     | 0.05        | 1         |
| B     | 115 | GLU  | HG3  | 2.1355     | 0.02        | 2         |
| B     | 93  | LEU  | HD22 | 0.93       | 0.02        | 2         |
| B     | 93  | LEU  | C    | 178.605    | 0.05        | 1         |
| A     | 100 | THR  | HG23 | 1.3291     | 0.02        | 1         |
| B     | 64  | ASP  | H    | 8.028      | 0.02        | 1         |
| B     | 103 | GLU  | N    | 122.544    | 0.05        | 1         |
| A     | 82  | MET  | C    | 176.221    | 0.05        | 1         |
| B     | 92  | LYS  | H    | 8.098      | 0.02        | 1         |
| B     | 102 | THR  | H    | 7.8492     | 0.02        | 1         |
| A     | 76  | GLY  | N    | 127.652    | 0.05        | 1         |
| A     | 68  | SER  | N    | 132.064    | 0.05        | 1         |
| B     | 109 | ALA  | HB1  | 1.5713     | 0.02        | 1         |
| A     | 74  | PHE  | HD2  | 7.1489     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 70  | LEU  | CD1  | 26.747     | 0.05        | 2         |
| B     | 88  | MET  | H    | 8.2253     | 0.02        | 1         |
| A     | 73  | ARG  | CB   | 30.439     | 0.05        | 1         |
| A     | 95  | ARG  | HG3  | 1.582      | 0.02        | 2         |
| A     | 66  | LEU  | HA   | 4.0843     | 0.02        | 1         |
| B     | 89  | THR  | HB   | 4.222      | 0.02        | 1         |
| A     | 107 | VAL  | HG21 | 1.0954     | 0.02        | 2         |
| B     | 67  | PHE  | HD2  | 6.6752     | 0.02        | 1         |
| A     | 113 | GLU  | CG   | 33.981     | 0.05        | 1         |
| A     | 96  | TYR  | HA   | 4.1779     | 0.02        | 1         |
| A     | 64  | ASP  | N    | 116.823    | 0.05        | 1         |
| B     | 110 | ARG  | CB   | 29.828     | 0.05        | 1         |
| B     | 119 | GLY  | HA2  | 3.9922     | 0.02        | 1         |
| A     | 80  | LEU  | HB2  | 1.553      | 0.02        | 2         |
| A     | 77  | GLY  | HA3  | 4.0045     | 0.02        | 1         |
| B     | 103 | GLU  | HG3  | 2.315      | 0.02        | 2         |
| A     | 85  | ASP  | HB3  | 2.692      | 0.02        | 1         |
| B     | 62  | SER  | H    | 8.4597     | 0.02        | 1         |
| A     | 97  | LEU  | HD22 | 1.0221     | 0.02        | 1         |
| B     | 107 | VAL  | C    | 177.9      | 0.05        | 1         |
| B     | 113 | GLU  | HB2  | 2.247      | 0.02        | 1         |
| A     | 115 | GLU  | CA   | 58.678     | 0.05        | 1         |
| A     | 74  | PHE  | CD2  | 131.005    | 0.05        | 1         |
| A     | 107 | VAL  | C    | 177.9      | 0.05        | 1         |
| A     | 118 | ALA  | CB   | 19.104     | 0.05        | 1         |
| B     | 114 | VAL  | HB   | 2.2135     | 0.02        | 1         |
| A     | 107 | VAL  | HG11 | 1.2189     | 0.02        | 2         |
| B     | 107 | VAL  | HG23 | 1.0954     | 0.02        | 2         |
| A     | 104 | LEU  | HD11 | 1.1055     | 0.02        | 2         |
| A     | 65  | GLU  | CB   | 29.5665    | 0.05        | 1         |
| B     | 98  | LYS  | HA   | 3.8503     | 0.02        | 1         |
| A     | 106 | SER  | HB3  | 4.0958     | 0.02        | 2         |
| A     | 105 | ASP  | HB3  | 2.6896     | 0.02        | 2         |
| B     | 97  | LEU  | HB3  | 1.6333     | 0.02        | 1         |
| B     | 92  | LYS  | CB   | 33.037     | 0.05        | 1         |
| B     | 107 | VAL  | CB   | 31.72      | 0.05        | 1         |
| A     | 101 | VAL  | HG11 | 1.1774     | 0.02        | 2         |
| A     | 67  | PHE  | N    | 116.555    | 0.05        | 1         |
| A     | 82  | MET  | HA   | 4.486      | 0.02        | 1         |
| A     | 105 | ASP  | HA   | 4.5076     | 0.02        | 1         |
| A     | 86  | ASN  | ND2  | 112.62     | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 96  | TYR  | CD2  | 132.505    | 0.05        | 1         |
| B     | 103 | GLU  | HA   | 4.1932     | 0.02        | 1         |
| A     | 73  | ARG  | H    | 7.776      | 0.02        | 1         |
| A     | 70  | LEU  | HA   | 3.7548     | 0.02        | 1         |
| B     | 108 | THR  | CA   | 67.738     | 0.05        | 1         |
| A     | 107 | VAL  | H    | 8.7596     | 0.02        | 1         |
| A     | 99  | ARG  | N    | 117.877    | 0.05        | 1         |
| A     | 102 | THR  | CA   | 66.896     | 0.05        | 1         |
| B     | 71  | ASP  | HB3  | 2.6608     | 0.02        | 2         |
| A     | 92  | LYS  | H    | 8.098      | 0.02        | 1         |
| A     | 76  | GLY  | CA   | 45.48      | 0.05        | 1         |
| A     | 68  | SER  | HB2  | 3.9998     | 0.02        | 1         |
| B     | 107 | VAL  | HG11 | 1.2189     | 0.02        | 2         |
| B     | 97  | LEU  | HG   | 1.639      | 0.02        | 1         |
| A     | 64  | ASP  | HB3  | 2.5973     | 0.02        | 2         |
| A     | 116 | HIS  | HD2  | 7.2787     | 0.02        | 1         |
| B     | 109 | ALA  | CA   | 55.2767    | 0.05        | 1         |
| B     | 68  | SER  | HB3  | 3.9998     | 0.02        | 1         |
| B     | 112 | ARG  | CD   | 43.449     | 0.05        | 1         |
| A     | 95  | ARG  | HA   | 4.0225     | 0.02        | 1         |
| B     | 83  | SER  | CA   | 58.593     | 0.05        | 1         |
| B     | 98  | LYS  | CA   | 60.696     | 0.05        | 1         |
| B     | 78  | GLU  | HG2  | 2.2413     | 0.02        | 1         |
| A     | 96  | TYR  | HB3  | 2.9381     | 0.02        | 2         |
| A     | 116 | HIS  | N    | 117.217    | 0.05        | 1         |
| B     | 116 | HIS  | HA   | 4.6413     | 0.02        | 1         |
| B     | 70  | LEU  | HD23 | 0.8188     | 0.02        | 2         |
| B     | 117 | ARG  | HD2  | 3.244      | 0.02        | 1         |
| B     | 112 | ARG  | HA   | 4.1704     | 0.02        | 1         |
| B     | 72  | GLN  | HE22 | 6.85       | 0.02        | 2         |
| B     | 65  | GLU  | HB2  | 2.093      | 0.02        | 2         |
| A     | 114 | VAL  | HA   | 3.9892     | 0.02        | 1         |
| A     | 90  | GLU  | HB3  | 2.0393     | 0.02        | 2         |
| B     | 69  | MET  | HG3  | 2.5146     | 0.02        | 2         |
| A     | 100 | THR  | HB   | 3.9695     | 0.02        | 1         |
| B     | 104 | LEU  | HD22 | 0.9838     | 0.02        | 2         |
| B     | 113 | GLU  | C    | 178.913    | 0.05        | 1         |
| B     | 64  | ASP  | C    | 179.052    | 0.05        | 1         |
| A     | 116 | HIS  | C    | 175.353    | 0.05        | 1         |
| B     | 106 | SER  | HB3  | 4.0958     | 0.02        | 2         |
| A     | 81  | LEU  | H    | 8.0625     | 0.02        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| A     | 93  | LEU  | HD21 | 0.93       | 0.02        | 2         |
| B     | 74  | PHE  | N    | 115.746    | 0.05        | 1         |
| A     | 74  | PHE  | HA   | 5.0077     | 0.02        | 1         |
| B     | 90  | GLU  | CB   | 29.8281    | 0.05        | 1         |
| B     | 100 | THR  | CA   | 67.753     | 0.05        | 1         |
| B     | 70  | LEU  | HD13 | 0.9524     | 0.02        | 2         |
| B     | 120 | GLU  | HA   | 4.171      | 0.02        | 1         |
| B     | 104 | LEU  | HD11 | 1.1055     | 0.02        | 2         |
| B     | 98  | LYS  | HB3  | 1.8925     | 0.02        | 1         |
| A     | 110 | ARG  | CD   | 43.36      | 0.05        | 1         |
| A     | 69  | MET  | CB   | 31.708     | 0.05        | 1         |
| A     | 101 | VAL  | HB   | 2.2517     | 0.02        | 1         |
| B     | 74  | PHE  | HZ   | 7.19       | 0.02        | 1         |
| B     | 64  | ASP  | HB3  | 2.5973     | 0.02        | 2         |
| B     | 69  | MET  | HB2  | 2.2694     | 0.02        | 1         |
| A     | 63  | ASP  | N    | 122.743    | 0.05        | 1         |
| A     | 109 | ALA  | C    | 180.452    | 0.05        | 1         |
| B     | 113 | GLU  | HG2  | 2.5467     | 0.02        | 2         |
| B     | 91  | GLU  | N    | 116.636    | 0.05        | 1         |

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 194      | $-0.47 \pm 0.12$                | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 178      | $0.25 \pm 0.04$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 222      | $-0.55 \pm 0.12$                | Should be applied          |
| $^{15}\text{N}$        | 222      | $-0.01 \pm 0.16$                | None needed ( $< 0.5$ ppm) |

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 80%, i.e. 870 atoms were assigned a chemical shift out of a possible 1082. 10 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|---------------|---------------|-----------------|-----------------|
| Backbone  | 416/430 (97%) | 170/172 (99%) | 162/172 (94%)   | 84/86 (98%)     |
| Sidechain | 426/612 (70%) | 270/354 (76%) | 152/216 (70%)   | 4/42 (10%)      |

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|          | Total          | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|----------|----------------|----------------|-----------------|-----------------|
| Aromatic | 28/40 (70%)    | 12/20 (60%)    | 14/14 (100%)    | 2/6 (33%)       |
| Overall  | 870/1082 (80%) | 452/546 (83%)  | 328/402 (82%)   | 90/134 (67%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 1020 atoms were assigned a chemical shift out of a possible 1382. 10 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-----------------|----------------|-----------------|-----------------|
| Backbone  | 510/592 (86%)   | 210/236 (89%)  | 196/240 (82%)   | 104/116 (90%)   |
| Sidechain | 482/750 (64%)   | 312/436 (72%)  | 166/272 (61%)   | 4/42 (10%)      |
| Aromatic  | 28/40 (70%)     | 12/20 (60%)    | 14/14 (100%)    | 2/6 (33%)       |
| Overall   | 1020/1382 (74%) | 534/692 (77%)  | 376/526 (71%)   | 110/164 (67%)   |

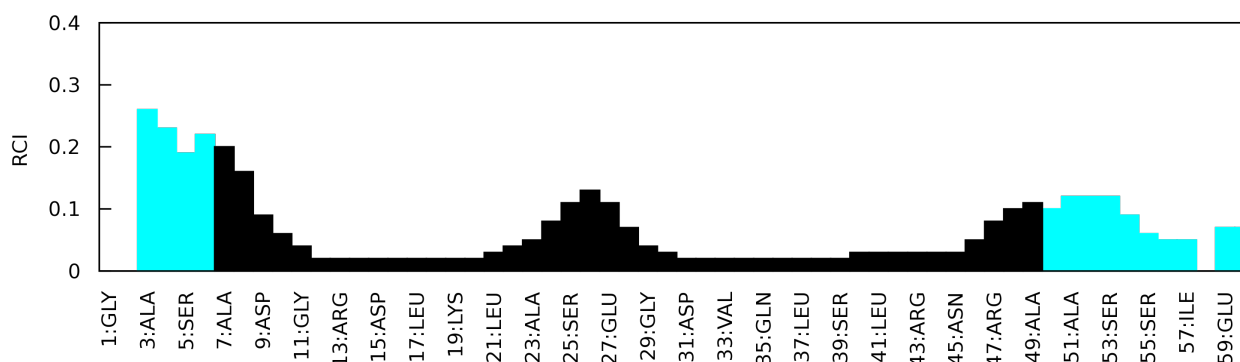
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The images below report *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:



Random coil index (RCI) for chain B:

