



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:34 pm BST

PDB ID : 2KKE  
Title : Solution NMR Structure of a dimeric protein of unknown function from Methanobacterium thermoautotrophicum, Northeast Structural Genomics Consortium Target TR5  
Authors : Swapna, G.V.T.; Gunsalus, X.; Huang, L.; Xiao, K.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2009-06-18

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

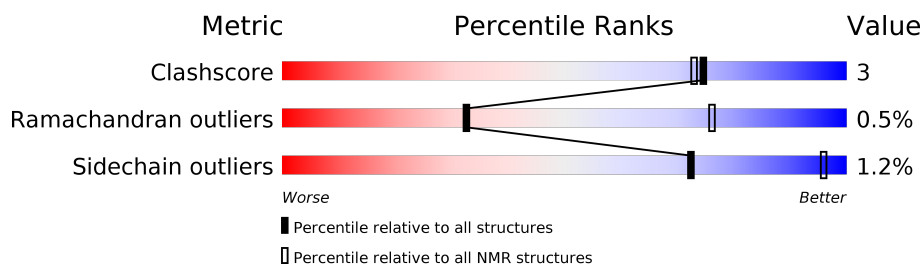
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 85%.

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            | 158937                      | 12864                     |
| Ramachandran outliers | 154571                      | 11451                     |
| Sidechain outliers    | 154315                      | 11428                     |

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     | 53     | <br>79% 21%      |
| 1   | B     | 53     | <br>79% 21%      |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                |                   |              |
|--------------------------------------|--------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)          | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:11-A:52, B:212-B:253<br>(84) | 0.53              | 5            |

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1711 atoms, of which 876 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |    |    |   | Trace |
|-----|-------|----------|-------|-----|-----|----|----|---|-------|
| 1   | A     | 53       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 856   | 261 | 439 | 78 | 76 | 2 |       |
| 1   | B     | 53       | Total | C   | H   | N  | O  | S | 0     |
|     |       |          | 855   | 261 | 437 | 78 | 77 | 2 |       |

There are 2 discrepancies between the modelled and reference sequences:

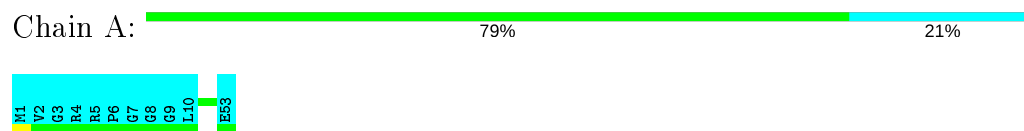
| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 53      | GLU      | ASP    | SEE REMARK 999 | UNP O26567 |
| B     | 253     | GLU      | ASP    | SEE REMARK 999 | UNP O26567 |

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

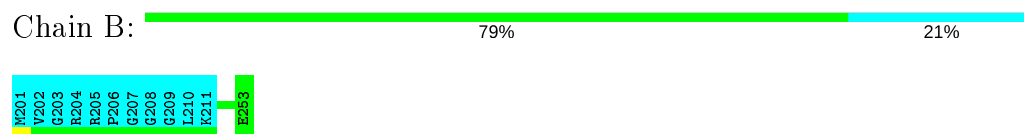
### 4.1 Average score per residue in the NMR ensemble

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: Uncharacterized protein



- Molecule 1: Uncharacterized protein

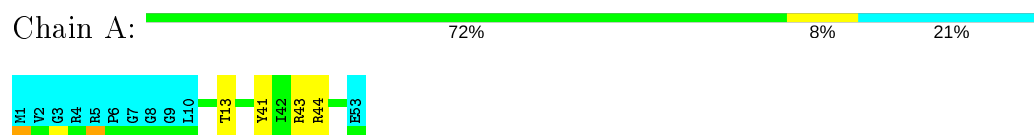


### 4.2 Scores per residue for each member of the ensemble

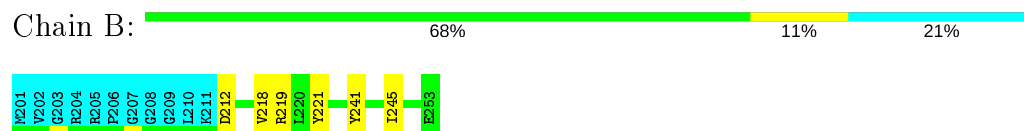
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Uncharacterized protein

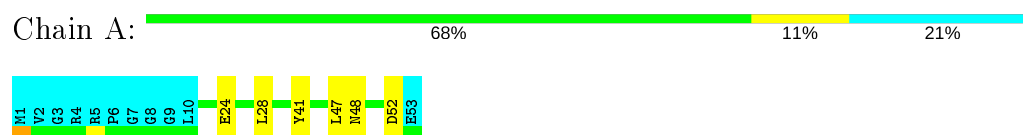


- Molecule 1: Uncharacterized protein

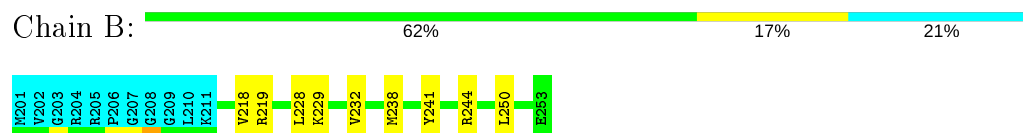


### 4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein

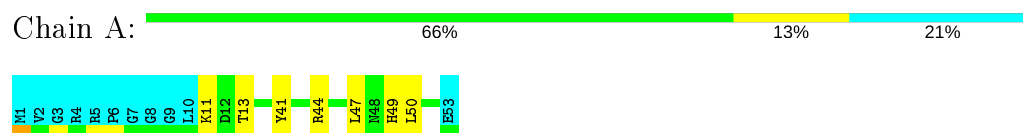


- Molecule 1: Uncharacterized protein



### 4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

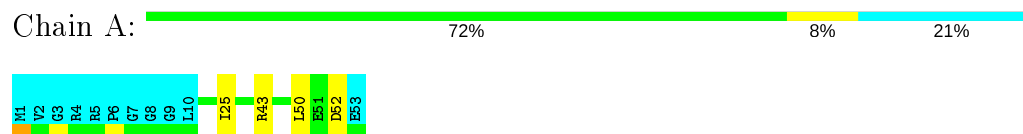


- Molecule 1: Uncharacterized protein

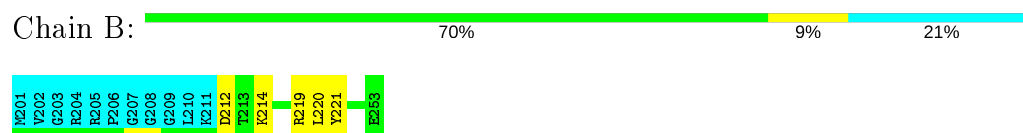


### 4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

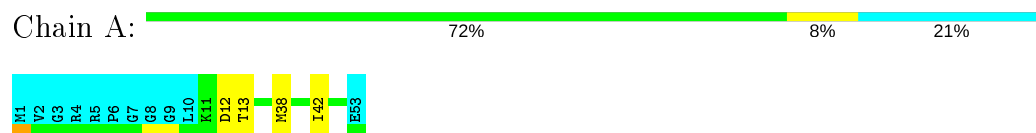


- Molecule 1: Uncharacterized protein

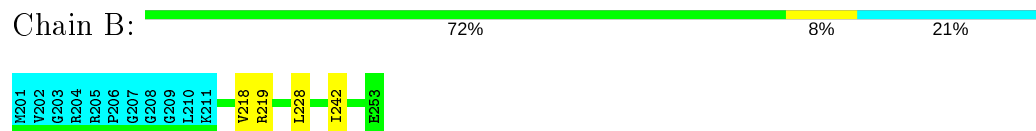


#### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Uncharacterized protein

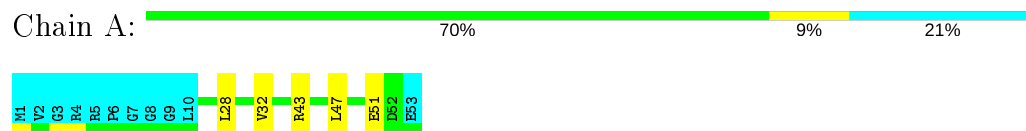


- Molecule 1: Uncharacterized protein

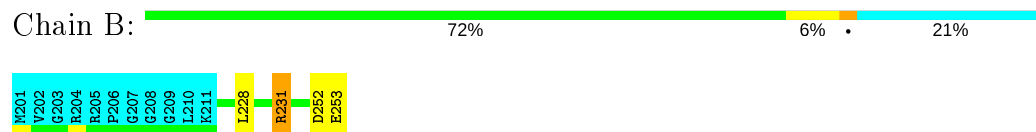


#### 4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein

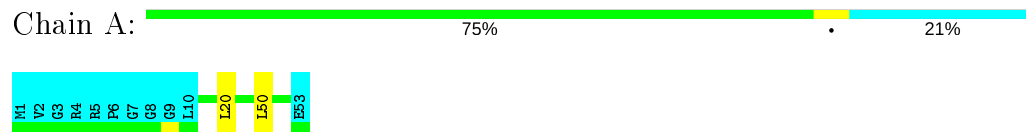


- Molecule 1: Uncharacterized protein

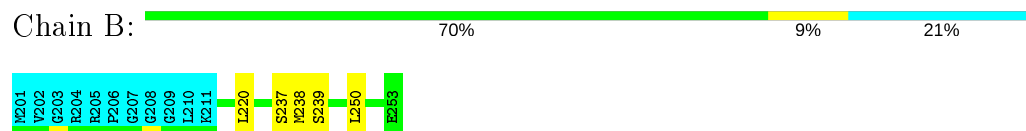


#### 4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein

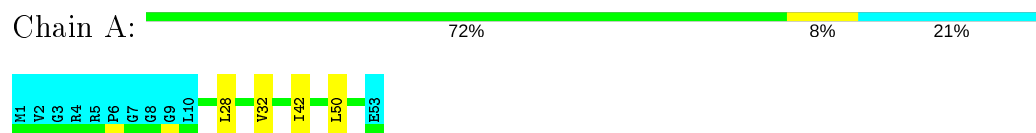


- Molecule 1: Uncharacterized protein

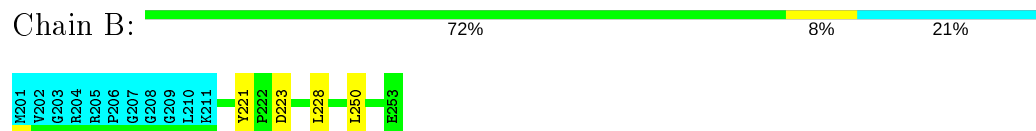


### 4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein

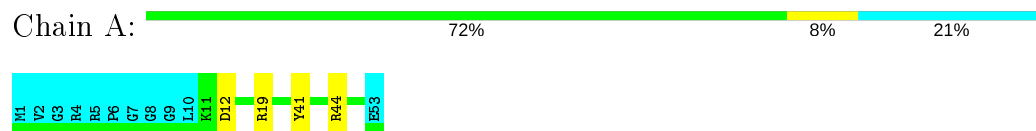


- Molecule 1: Uncharacterized protein

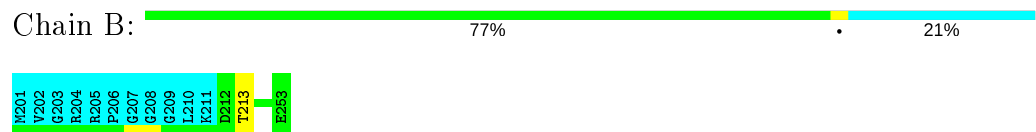


### 4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein

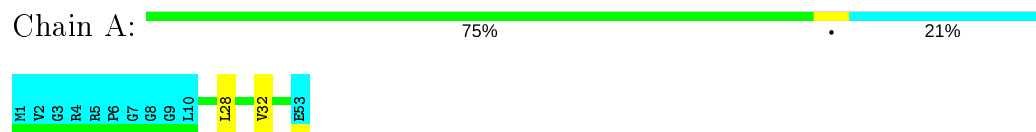


- Molecule 1: Uncharacterized protein

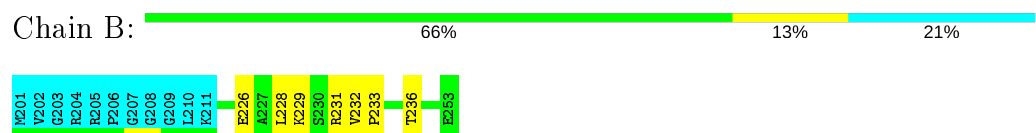


### 4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



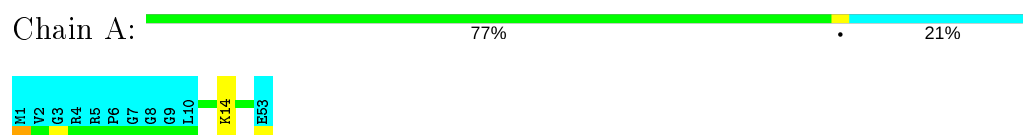
- Molecule 1: Uncharacterized protein





### 4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein

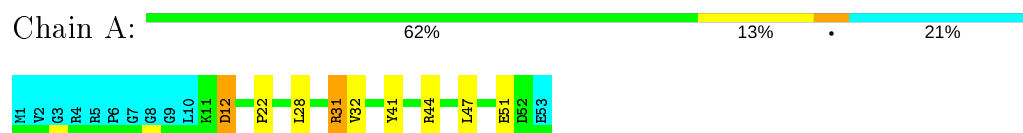


- Molecule 1: Uncharacterized protein

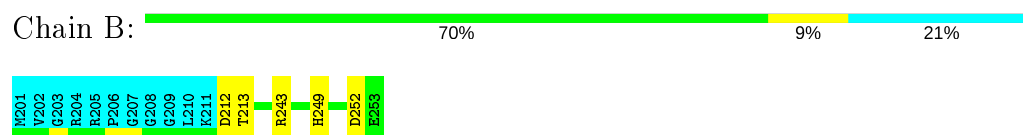


### 4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein

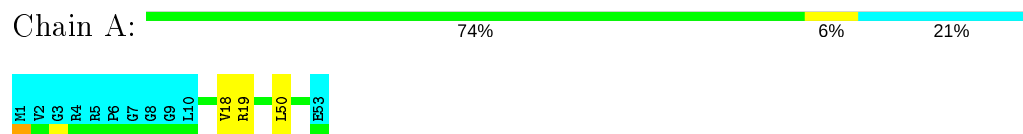


- Molecule 1: Uncharacterized protein

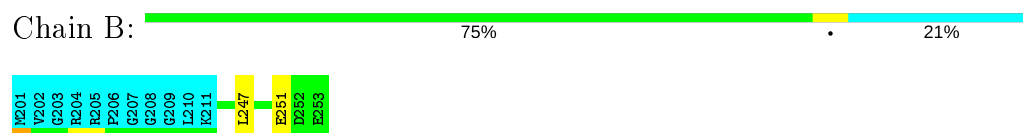


### 4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein

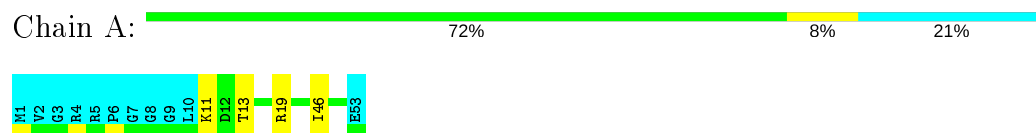


- Molecule 1: Uncharacterized protein

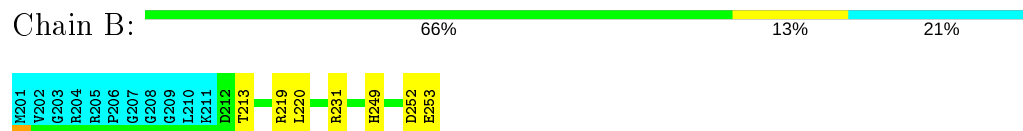


#### 4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein

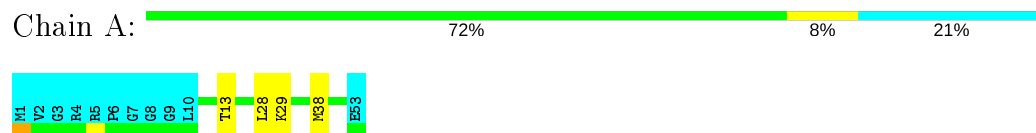


- Molecule 1: Uncharacterized protein

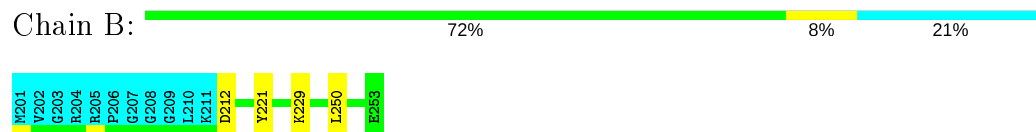


#### 4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein

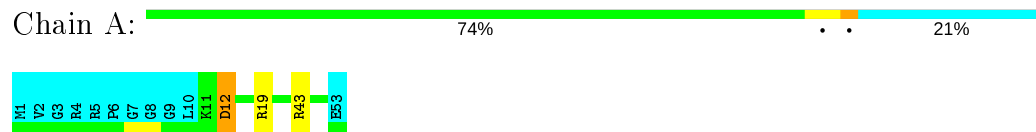


- Molecule 1: Uncharacterized protein

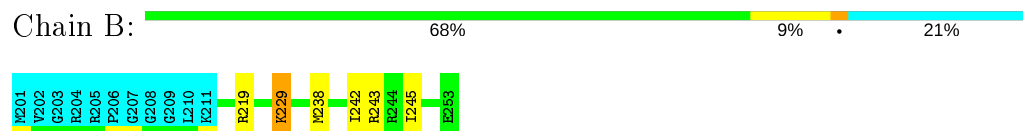


#### 4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein

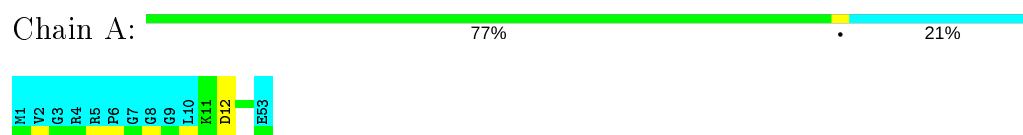


- Molecule 1: Uncharacterized protein

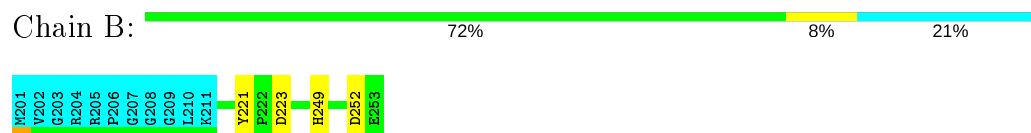


#### 4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein

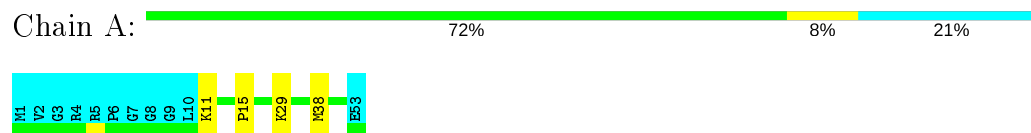


- Molecule 1: Uncharacterized protein

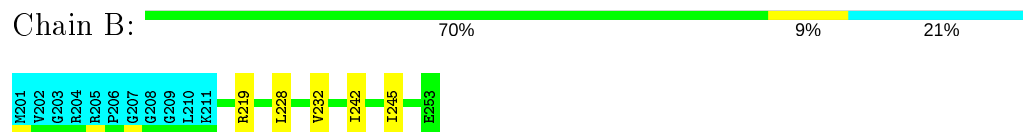


#### 4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein

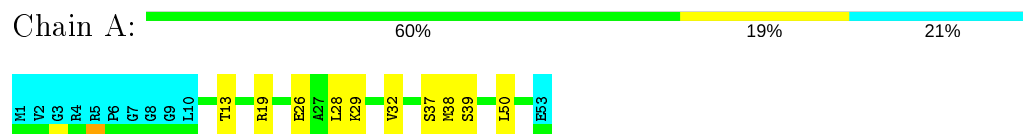


- Molecule 1: Uncharacterized protein

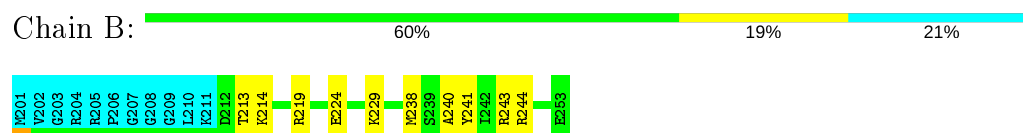


#### 4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein

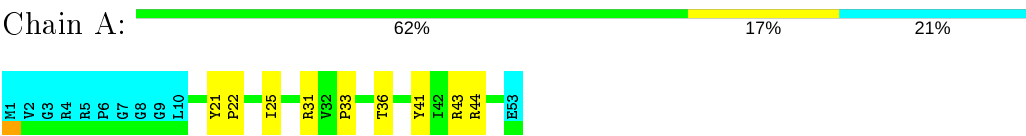


- Molecule 1: Uncharacterized protein

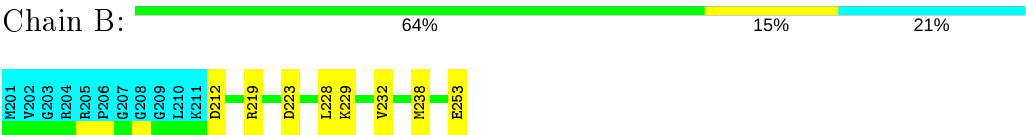


4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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 |
|---------------|-----------------------|---------|
| CYANA         | geometry optimization | 2.1     |
| CNS           | geometry optimization | 2.0.6   |
| CNS           | refinement            | 2.0.6   |

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)                       | input_cs.cif |
| Number of chemical shift lists               | 1            |
| Total number of shifts                       | 2568         |
| Number of shifts mapped to atoms             | 1284         |
| Number of unparsed shifts                    | 642          |
| Number of shifts with mapping errors         | 642          |
| Number of shifts with mapping warnings       | 0            |
| Assignment completeness (well-defined parts) | 85%          |

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     | 340   | 357      | 356      | 3±2     |
| 1   | B     | 341   | 350      | 349      | 3±2     |
| All | All   | 13620 | 14140    | 14100    | 88      |

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 3.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:24:GLU:HB3   | 1:B:250:LEU:HG   | 0.60     | 1.72        | 2      | 1     |
| 1:B:244:ARG:HA   | 1:B:247:LEU:HB3  | 0.57     | 1.77        | 3      | 1     |
| 1:A:13:THR:OG1   | 1:B:219:ARG:HB3  | 0.57     | 2.00        | 14     | 3     |
| 1:B:228:LEU:HD21 | 1:B:242:ILE:HD11 | 0.56     | 1.77        | 5      | 1     |
| 1:B:218:VAL:HG22 | 1:B:219:ARG:H    | 0.56     | 1.61        | 1      | 2     |
| 1:A:50:LEU:HD11  | 1:B:228:LEU:HB2  | 0.55     | 1.78        | 8      | 1     |
| 1:A:15:PRO:HA    | 1:B:219:ARG:HG2  | 0.54     | 1.80        | 18     | 1     |
| 1:B:229:LYS:HB3  | 1:B:238:MET:SD   | 0.53     | 2.43        | 16     | 3     |
| 1:A:13:THR:HG21  | 1:A:43:ARG:HD2   | 0.52     | 1.81        | 1      | 1     |
| 1:A:37:SER:O     | 1:A:39:SER:N     | 0.52     | 2.43        | 19     | 1     |
| 1:B:229:LYS:HE2  | 1:B:238:MET:SD   | 0.51     | 2.46        | 2      | 1     |
| 1:B:249:HIS:HA   | 1:B:252:ASP:HB3  | 0.51     | 1.82        | 17     | 3     |
| 1:A:33:PRO:HG2   | 1:A:36:THR:HB    | 0.51     | 1.83        | 20     | 1     |

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| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:41:TYR:O     | 1:A:44:ARG:HG2   | 0.49     | 2.07        | 3      | 5     |
| 1:B:242:ILE:HD13 | 1:B:245:ILE:HD12 | 0.49     | 1.84        | 18     | 3     |
| 1:A:50:LEU:HG    | 1:B:220:LEU:HD11 | 0.49     | 1.85        | 4      | 2     |
| 1:B:213:THR:HG21 | 1:B:243:ARG:HD2  | 0.49     | 1.84        | 12     | 1     |
| 1:A:19:ARG:HB3   | 1:B:213:THR:HB   | 0.48     | 1.85        | 19     | 2     |
| 1:A:29:LYS:HB3   | 1:A:38:MET:SD    | 0.48     | 2.48        | 15     | 2     |
| 1:B:229:LYS:HA   | 1:B:232:VAL:HG22 | 0.48     | 1.85        | 2      | 1     |
| 1:A:25:ILE:HD12  | 1:B:214:LYS:HB2  | 0.48     | 1.85        | 4      | 1     |
| 1:A:28:LEU:O     | 1:A:32:VAL:HG13  | 0.47     | 2.09        | 6      | 5     |
| 1:A:31:ARG:NH2   | 1:B:253:GLU:HG3  | 0.47     | 2.25        | 20     | 1     |
| 1:B:218:VAL:HG22 | 1:B:219:ARG:N    | 0.47     | 2.25        | 5      | 2     |
| 1:A:47:LEU:O     | 1:A:51:GLU:HG2   | 0.46     | 2.10        | 6      | 2     |
| 1:A:19:ARG:HB3   | 1:B:213:THR:OG1  | 0.46     | 2.11        | 14     | 1     |
| 1:A:11:LYS:O     | 1:A:11:LYS:HG3   | 0.45     | 2.11        | 3      | 1     |
| 1:A:13:THR:HB    | 1:B:219:ARG:HB3  | 0.44     | 1.90        | 19     | 1     |
| 1:B:228:LEU:O    | 1:B:232:VAL:HG13 | 0.44     | 2.12        | 2      | 5     |
| 1:B:241:TYR:O    | 1:B:244:ARG:HG2  | 0.44     | 2.12        | 19     | 2     |
| 1:B:226:GLU:HG3  | 1:B:229:LYS:HE2  | 0.44     | 1.89        | 10     | 1     |
| 1:A:13:THR:HG22  | 1:B:221:TYR:HA   | 0.44     | 1.89        | 15     | 1     |
| 1:A:49:HIS:HD2   | 1:B:245:ILE:HG23 | 0.44     | 1.73        | 3      | 1     |
| 1:A:28:LEU:HD11  | 1:A:41:TYR:CE2   | 0.43     | 2.49        | 2      | 1     |
| 1:A:46:ILE:HD12  | 1:B:220:LEU:HD13 | 0.43     | 1.90        | 14     | 1     |
| 1:A:38:MET:O     | 1:A:42:ILE:HG12  | 0.43     | 2.14        | 5      | 1     |
| 1:A:43:ARG:HG3   | 1:B:219:ARG:O    | 0.43     | 2.14        | 16     | 1     |
| 1:B:247:LEU:O    | 1:B:251:GLU:HG2  | 0.43     | 2.13        | 13     | 1     |
| 1:A:50:LEU:HG    | 1:B:220:LEU:HD21 | 0.43     | 1.91        | 7      | 1     |
| 1:A:28:LEU:HD21  | 1:A:42:ILE:HD11  | 0.42     | 1.92        | 8      | 1     |
| 1:A:43:ARG:O     | 1:A:47:LEU:HD13  | 0.42     | 2.15        | 6      | 1     |
| 1:B:237:SER:O    | 1:B:239:SER:N    | 0.42     | 2.53        | 11     | 2     |
| 1:A:28:LEU:O     | 1:A:31:ARG:HG2   | 0.42     | 2.13        | 12     | 1     |
| 1:B:233:PRO:HG2  | 1:B:236:THR:HB   | 0.42     | 1.91        | 10     | 1     |
| 1:A:43:ARG:HD3   | 1:B:219:ARG:HB2  | 0.42     | 1.90        | 4      | 2     |
| 1:A:21:TYR:O     | 1:A:25:ILE:HG13  | 0.42     | 2.14        | 20     | 1     |
| 1:B:228:LEU:HD12 | 1:B:231:ARG:HH21 | 0.41     | 1.75        | 6      | 1     |
| 1:A:19:ARG:O     | 1:B:243:ARG:HG3  | 0.41     | 2.15        | 16     | 1     |
| 1:A:48:ASN:O     | 1:A:52:ASP:HB2   | 0.41     | 2.16        | 2      | 1     |
| 1:A:28:LEU:HD13  | 1:B:250:LEU:HD11 | 0.41     | 1.91        | 8      | 1     |
| 1:A:18:VAL:HG12  | 1:A:19:ARG:N     | 0.41     | 2.30        | 13     | 1     |
| 1:A:28:LEU:HB2   | 1:B:250:LEU:HD11 | 0.41     | 1.91        | 15     | 1     |
| 1:A:20:LEU:HD21  | 1:B:250:LEU:HG   | 0.41     | 1.93        | 7      | 1     |
| 1:A:50:LEU:HB3   | 1:B:224:GLU:HB3  | 0.41     | 1.93        | 19     | 1     |

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| Atom-1          | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|-----------------|------------------|----------|-------------|--------|-------|
|                 |                  |          |             | Worst  | Total |
| 1:B:241:TYR:O   | 1:B:245:ILE:HG13 | 0.40     | 2.16        | 1      | 1     |
| 1:B:252:ASP:O   | 1:B:253:GLU:HG2  | 0.40     | 2.17        | 6      | 1     |
| 1:B:231:ARG:NH2 | 1:B:241:TYR:OH   | 0.40     | 2.53        | 11     | 1     |
| 1:A:26:GLU:HA   | 1:A:29:LYS:HG2   | 0.40     | 1.94        | 19     | 1     |
| 1:B:240:ALA:O   | 1:B:243:ARG:HB3  | 0.40     | 2.17        | 19     | 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     | 42/53 (79%)     | 39±2 (93±4%) | 3±2 (6±4%) | 0±0 (0±1%) | 32          | 76 |
| 1   | B     | 41/53 (77%)     | 39±1 (94±3%) | 2±1 (5±3%) | 0±0 (0±1%) | 32          | 76 |
| All | All   | 1660/2120 (78%) | 1555 (94%)   | 97 (6%)    | 8 (0%)     | 32          | 76 |

All 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | B     | 238 | MET  | 2              |
| 1   | A     | 12  | ASP  | 1              |
| 1   | A     | 52  | ASP  | 1              |
| 1   | B     | 231 | ARG  | 1              |
| 1   | B     | 212 | ASP  | 1              |
| 1   | A     | 22  | PRO  | 1              |
| 1   | A     | 38  | MET  | 1              |

### 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     | 39/46 (85%)     | 39±1 (99±1%) | 0±1 (1±1%) | 82          | 97 |
| 1   | B     | 39/46 (85%)     | 38±1 (98±2%) | 1±1 (2±2%) | 62          | 94 |
| All | All   | 1560/1840 (85%) | 1541 (99%)   | 19 (1%)    | 72          | 96 |

All 12 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   | B     | 212 | ASP  | 5              |
| 1   | A     | 12  | ASP  | 2              |
| 1   | B     | 223 | ASP  | 2              |
| 1   | B     | 229 | LYS  | 2              |
| 1   | A     | 14  | LYS  | 1              |
| 1   | B     | 244 | ARG  | 1              |
| 1   | A     | 11  | LYS  | 1              |
| 1   | A     | 50  | LEU  | 1              |
| 1   | A     | 31  | ARG  | 1              |
| 1   | B     | 214 | LYS  | 1              |
| 1   | B     | 253 | GLU  | 1              |
| 1   | B     | 231 | 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 85% for the well-defined parts and 84% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

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

#### 7.1.1 Bookkeeping

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

|   |      |
|---|------|
| Total number of shifts                  | 2568 |
| Number of shifts mapped to atoms        | 1284 |
| Number of unparsed shifts               | 642  |
| Number of shifts with mapping errors    | 642  |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 642 occurrences are reported below.

| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1285     | A     | 1   | MET  | HA   | 4.562      | 0.05        | 1         |
| 1287     | A     | 1   | MET  | HB2  | 2.060      | 0.05        | 2         |
| 1289     | A     | 1   | MET  | HB3  | 2.147      | 0.05        | 2         |
| 1291     | A     | 1   | MET  | HE1  | 2.166      | 0.05        | 1         |
| 1293     | A     | 1   | MET  | HE2  | 2.166      | 0.05        | 1         |
| 1295     | A     | 1   | MET  | HE3  | 2.166      | 0.05        | 1         |
| 1297     | A     | 1   | MET  | HG2  | 2.53       | 0.05        | 2         |
| 1299     | A     | 1   | MET  | HG3  | 2.61       | 0.05        | 2         |
| 1301     | A     | 1   | MET  | C    | 176.534    | 0.3         | 1         |
| 1303     | A     | 1   | MET  | CA   | 55.75      | 0.3         | 1         |
| 1305     | A     | 1   | MET  | CB   | 33.026     | 0.3         | 1         |
| 1307     | A     | 1   | MET  | CE   | 17.265     | 0.3         | 1         |
| 1309     | A     | 1   | MET  | CG   | 32.138     | 0.3         | 1         |
| 1311     | A     | 2   | VAL  | H    | 8.215      | 0.05        | 1         |
| 1313     | A     | 2   | VAL  | HA   | 4.189      | 0.05        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1315     | A     | 2   | VAL  | HB   | 2.16       | 0.05        | 1         |
| 1317     | A     | 2   | VAL  | HG11 | 1.037      | 0.05        | 2         |
| 1319     | A     | 2   | VAL  | HG12 | 1.037      | 0.05        | 2         |
| 1321     | A     | 2   | VAL  | HG13 | 1.037      | 0.05        | 2         |
| 1323     | A     | 2   | VAL  | HG21 | 1.037      | 0.05        | 2         |
| 1325     | A     | 2   | VAL  | HG22 | 1.037      | 0.05        | 2         |
| 1327     | A     | 2   | VAL  | HG23 | 1.037      | 0.05        | 2         |
| 1329     | A     | 2   | VAL  | C    | 177.021    | 0.3         | 1         |
| 1331     | A     | 2   | VAL  | CA   | 62.709     | 0.3         | 1         |
| 1333     | A     | 2   | VAL  | CB   | 32.822     | 0.3         | 1         |
| 1335     | A     | 2   | VAL  | CG1  | 21.0       | 0.3         | 2         |
| 1337     | A     | 2   | VAL  | CG2  | 21.0       | 0.3         | 2         |
| 1339     | A     | 2   | VAL  | N    | 121.358    | 0.3         | 1         |
| 1341     | A     | 3   | GLY  | H    | 8.55       | 0.05        | 1         |
| 1343     | A     | 3   | GLY  | HA2  | 4.051      | 0.05        | 2         |
| 1345     | A     | 3   | GLY  | HA3  | 4.05       | 0.05        | 2         |
| 1347     | A     | 3   | GLY  | CA   | 45.39      | 0.3         | 1         |
| 1349     | A     | 3   | GLY  | N    | 112.524    | 0.3         | 1         |
| 1351     | A     | 4   | ARG  | H    | 8.159      | 0.05        | 1         |
| 1353     | A     | 4   | ARG  | HA   | 4.44       | 0.05        | 1         |
| 1355     | A     | 4   | ARG  | HB2  | 1.900      | 0.05        | 2         |
| 1357     | A     | 4   | ARG  | HB3  | 1.838      | 0.05        | 2         |
| 1359     | A     | 4   | ARG  | HD2  | 3.224      | 0.05        | 2         |
| 1361     | A     | 4   | ARG  | HD3  | 3.224      | 0.05        | 2         |
| 1363     | A     | 4   | ARG  | HG2  | 1.665      | 0.05        | 2         |
| 1365     | A     | 4   | ARG  | HG3  | 1.665      | 0.05        | 2         |
| 1367     | A     | 4   | ARG  | C    | 176.599    | 0.3         | 1         |
| 1369     | A     | 4   | ARG  | CA   | 55.82      | 0.3         | 1         |
| 1371     | A     | 4   | ARG  | CB   | 31.179     | 0.3         | 1         |
| 1373     | A     | 4   | ARG  | CD   | 43.419     | 0.3         | 1         |
| 1375     | A     | 4   | ARG  | CG   | 27.15      | 0.3         | 1         |
| 1377     | A     | 4   | ARG  | N    | 120.490    | 0.3         | 1         |
| 1379     | A     | 5   | ARG  | H    | 8.522      | 0.05        | 1         |
| 1381     | A     | 5   | ARG  | HA   | 4.594      | 0.05        | 1         |
| 1383     | A     | 5   | ARG  | HB2  | 2.007      | 0.05        | 2         |
| 1385     | A     | 5   | ARG  | HB3  | 2.081      | 0.05        | 2         |
| 1387     | A     | 5   | ARG  | HD2  | 3.354      | 0.05        | 2         |
| 1389     | A     | 5   | ARG  | CB   | 29.728     | 0.3         | 1         |
| 1391     | A     | 5   | ARG  | CD   | 43.676     | 0.3         | 1         |
| 1393     | A     | 5   | ARG  | CG   | 26.489     | 0.3         | 1         |
| 1395     | A     | 5   | ARG  | N    | 123.728    | 0.3         | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1397     | A     | 6   | PRO  | HA   | 4.550      | 0.05        | 1         |
| 1399     | A     | 6   | PRO  | HB2  | 2.054      | 0.05        | 2         |
| 1401     | A     | 6   | PRO  | HB3  | 2.408      | 0.05        | 2         |
| 1403     | A     | 6   | PRO  | HD2  | 4.330      | 0.05        | 2         |
| 1405     | A     | 6   | PRO  | HD3  | 4.204      | 0.05        | 2         |
| 1407     | A     | 6   | PRO  | HG2  | 2.05       | 0.05        | 2         |
| 1409     | A     | 6   | PRO  | HG3  | 2.05       | 0.05        | 2         |
| 1411     | A     | 6   | PRO  | C    | 178.098    | 0.3         | 1         |
| 1413     | A     | 6   | PRO  | CA   | 63.632     | 0.3         | 1         |
| 1415     | A     | 6   | PRO  | CB   | 32.259     | 0.3         | 1         |
| 1417     | A     | 6   | PRO  | CD   | 50.879     | 0.3         | 1         |
| 1419     | A     | 6   | PRO  | CG   | 27.751     | 0.3         | 1         |
| 1421     | A     | 7   | GLY  | H    | 8.615      | 0.05        | 1         |
| 1423     | A     | 7   | GLY  | HA2  | 4.09       | 0.05        | 2         |
| 1425     | A     | 7   | GLY  | HA3  | 4.09       | 0.05        | 2         |
| 1427     | A     | 7   | GLY  | C    | 175.353    | 0.3         | 1         |
| 1429     | A     | 7   | GLY  | CA   | 45.26      | 0.3         | 1         |
| 1431     | A     | 7   | GLY  | N    | 109.847    | 0.3         | 1         |
| 1433     | A     | 8   | GLY  | H    | 8.382      | 0.05        | 1         |
| 1435     | A     | 8   | GLY  | HA2  | 4.07       | 0.05        | 2         |
| 1437     | A     | 8   | GLY  | HA3  | 4.13       | 0.05        | 2         |
| 1439     | A     | 8   | GLY  | C    | 175.236    | 0.3         | 1         |
| 1441     | A     | 8   | GLY  | CA   | 45.46      | 0.3         | 1         |
| 1443     | A     | 8   | GLY  | N    | 108.964    | 0.3         | 1         |
| 1445     | A     | 9   | GLY  | H    | 8.533      | 0.05        | 1         |
| 1447     | A     | 9   | GLY  | HA2  | 4.03       | 0.05        | 2         |
| 1449     | A     | 9   | GLY  | HA3  | 4.03       | 0.05        | 2         |
| 1451     | A     | 9   | GLY  | CA   | 45.5       | 0.3         | 1         |
| 1453     | A     | 9   | GLY  | N    | 109.175    | 0.3         | 1         |
| 1455     | A     | 10  | LEU  | H    | 8.328      | 0.05        | 1         |
| 1457     | A     | 10  | LEU  | HA   | 4.312      | 0.05        | 1         |
| 1459     | A     | 10  | LEU  | HB2  | 1.762      | 0.05        | 2         |
| 1461     | A     | 10  | LEU  | HB3  | 1.647      | 0.05        | 2         |
| 1463     | A     | 10  | LEU  | HD11 | 0.98       | 0.05        | 2         |
| 1465     | A     | 10  | LEU  | HD12 | 0.98       | 0.05        | 2         |
| 1467     | A     | 10  | LEU  | HD13 | 0.98       | 0.05        | 2         |
| 1469     | A     | 10  | LEU  | HD21 | 0.907      | 0.05        | 2         |
| 1471     | A     | 10  | LEU  | HD22 | 0.907      | 0.05        | 2         |
| 1473     | A     | 10  | LEU  | HD23 | 0.907      | 0.05        | 2         |
| 1475     | A     | 10  | LEU  | HG   | 1.712      | 0.05        | 1         |
| 1477     | A     | 10  | LEU  | CA   | 56.244     | 0.3         | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1479     | A     | 10  | LEU  | CB   | 42.353     | 0.3         | 1         |
| 1481     | A     | 10  | LEU  | CD1  | 25.09      | 0.3         | 2         |
| 1483     | A     | 10  | LEU  | CD2  | 23.3       | 0.3         | 2         |
| 1485     | A     | 10  | LEU  | CG   | 27.117     | 0.3         | 1         |
| 1487     | A     | 10  | LEU  | N    | 121.467    | 0.3         | 1         |
| 1489     | A     | 11  | LYS  | H    | 8.354      | 0.05        | 1         |
| 1491     | A     | 11  | LYS  | HA   | 4.415      | 0.05        | 1         |
| 1493     | A     | 11  | LYS  | HB2  | 1.93       | 0.05        | 2         |
| 1495     | A     | 11  | LYS  | HB3  | 1.99       | 0.05        | 2         |
| 1497     | A     | 11  | LYS  | HD2  | 1.778      | 0.05        | 2         |
| 1499     | A     | 11  | LYS  | HD3  | 1.778      | 0.05        | 2         |
| 1501     | A     | 11  | LYS  | HE2  | 3.08       | 0.05        | 2         |
| 1503     | A     | 11  | LYS  | HE3  | 3.080      | 0.05        | 2         |
| 1505     | A     | 11  | LYS  | HG2  | 1.550      | 0.05        | 2         |
| 1507     | A     | 11  | LYS  | HG3  | 1.550      | 0.05        | 2         |
| 1509     | A     | 11  | LYS  | CA   | 57.220     | 0.3         | 1         |
| 1511     | A     | 11  | LYS  | CB   | 32.929     | 0.3         | 1         |
| 1513     | A     | 11  | LYS  | CD   | 29.350     | 0.3         | 1         |
| 1515     | A     | 11  | LYS  | CE   | 42.421     | 0.3         | 1         |
| 1517     | A     | 11  | LYS  | CG   | 24.870     | 0.3         | 1         |
| 1519     | A     | 11  | LYS  | N    | 119.917    | 0.3         | 1         |
| 1521     | A     | 12  | ASP  | H    | 8.187      | 0.05        | 1         |
| 1523     | A     | 12  | ASP  | HA   | 4.85       | 0.05        | 1         |
| 1525     | A     | 12  | ASP  | HB2  | 2.86       | 0.05        | 2         |
| 1527     | A     | 12  | ASP  | HB3  | 3.01       | 0.05        | 2         |
| 1529     | A     | 12  | ASP  | C    | 176.436    | 0.3         | 1         |
| 1531     | A     | 12  | ASP  | CA   | 54.4       | 0.3         | 1         |
| 1533     | A     | 12  | ASP  | CB   | 41.82      | 0.3         | 1         |
| 1535     | A     | 12  | ASP  | N    | 118.931    | 0.3         | 1         |
| 1537     | A     | 13  | THR  | H    | 7.615      | 0.05        | 1         |
| 1539     | A     | 13  | THR  | HA   | 4.256      | 0.05        | 1         |
| 1541     | A     | 13  | THR  | HB   | 3.681      | 0.05        | 1         |
| 1543     | A     | 13  | THR  | HG21 | 0.317      | 0.05        | 1         |
| 1545     | A     | 13  | THR  | HG22 | 0.317      | 0.05        | 1         |
| 1547     | A     | 13  | THR  | HG23 | 0.317      | 0.05        | 1         |
| 1549     | A     | 13  | THR  | CA   | 60.358     | 0.3         | 1         |
| 1551     | A     | 13  | THR  | CB   | 72.453     | 0.3         | 1         |
| 1553     | A     | 13  | THR  | CG2  | 20.656     | 0.3         | 1         |
| 1555     | A     | 13  | THR  | N    | 107.789    | 0.3         | 1         |
| 1557     | A     | 14  | LYS  | H    | 9.064      | 0.05        | 1         |
| 1559     | A     | 14  | LYS  | HA   | 4.952      | 0.05        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1561     | A     | 14  | LYS  | HB2  | 1.909      | 0.05        | 2         |
| 1563     | A     | 14  | LYS  | HB3  | 1.657      | 0.05        | 2         |
| 1565     | A     | 14  | LYS  | HD2  | 1.780      | 0.05        | 2         |
| 1567     | A     | 14  | LYS  | HD3  | 1.775      | 0.05        | 2         |
| 1569     | A     | 14  | LYS  | HE2  | 3.119      | 0.05        | 2         |
| 1571     | A     | 14  | LYS  | HE3  | 3.059      | 0.05        | 2         |
| 1573     | A     | 14  | LYS  | HG2  | 1.563      | 0.05        | 2         |
| 1575     | A     | 14  | LYS  | HG3  | 1.465      | 0.05        | 2         |
| 1577     | A     | 14  | LYS  | CA   | 52.486     | 0.3         | 1         |
| 1579     | A     | 14  | LYS  | CB   | 34.372     | 0.3         | 1         |
| 1581     | A     | 14  | LYS  | CD   | 29.114     | 0.3         | 1         |
| 1583     | A     | 14  | LYS  | CE   | 42.416     | 0.3         | 1         |
| 1585     | A     | 14  | LYS  | CG   | 24.732     | 0.3         | 1         |
| 1587     | A     | 14  | LYS  | N    | 119.891    | 0.3         | 1         |
| 1589     | A     | 15  | PRO  | HB2  | 1.867      | 0.05        | 2         |
| 1591     | A     | 15  | PRO  | HB3  | 1.932      | 0.05        | 2         |
| 1593     | A     | 15  | PRO  | HD2  | 3.747      | 0.05        | 2         |
| 1595     | A     | 15  | PRO  | HD3  | 3.861      | 0.05        | 2         |
| 1597     | A     | 15  | PRO  | HG2  | 2.325      | 0.05        | 2         |
| 1599     | A     | 15  | PRO  | HG3  | 2.130      | 0.05        | 2         |
| 1601     | A     | 15  | PRO  | C    | 177.155    | 0.3         | 1         |
| 1603     | A     | 15  | PRO  | CA   | 62.351     | 0.3         | 1         |
| 1605     | A     | 15  | PRO  | CB   | 33.036     | 0.3         | 1         |
| 1607     | A     | 15  | PRO  | CD   | 50.446     | 0.3         | 1         |
| 1609     | A     | 15  | PRO  | CG   | 26.933     | 0.3         | 1         |
| 1611     | A     | 16  | VAL  | H    | 9.112      | 0.05        | 1         |
| 1613     | A     | 16  | VAL  | HA   | 4.29       | 0.05        | 1         |
| 1615     | A     | 16  | VAL  | HB   | 2.054      | 0.05        | 1         |
| 1617     | A     | 16  | VAL  | HG11 | 0.902      | 0.05        | 2         |
| 1619     | A     | 16  | VAL  | HG12 | 0.902      | 0.05        | 2         |
| 1621     | A     | 16  | VAL  | HG13 | 0.902      | 0.05        | 2         |
| 1623     | A     | 16  | VAL  | HG21 | 0.865      | 0.05        | 2         |
| 1625     | A     | 16  | VAL  | HG22 | 0.865      | 0.05        | 2         |
| 1627     | A     | 16  | VAL  | HG23 | 0.865      | 0.05        | 2         |
| 1629     | A     | 16  | VAL  | C    | 174.696    | 0.3         | 1         |
| 1631     | A     | 16  | VAL  | CA   | 61.845     | 0.3         | 1         |
| 1633     | A     | 16  | VAL  | CB   | 34.265     | 0.3         | 1         |
| 1635     | A     | 16  | VAL  | CG1  | 21.088     | 0.3         | 2         |
| 1637     | A     | 16  | VAL  | CG2  | 21.156     | 0.3         | 2         |
| 1639     | A     | 16  | VAL  | N    | 124.670    | 0.3         | 1         |
| 1641     | A     | 17  | VAL  | H    | 8.338      | 0.05        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1643     | A     | 17  | VAL  | HA   | 4.496      | 0.05        | 1         |
| 1645     | A     | 17  | VAL  | HB   | 1.994      | 0.05        | 1         |
| 1647     | A     | 17  | VAL  | HG11 | 0.830      | 0.05        | 2         |
| 1649     | A     | 17  | VAL  | HG12 | 0.830      | 0.05        | 2         |
| 1651     | A     | 17  | VAL  | HG13 | 0.830      | 0.05        | 2         |
| 1653     | A     | 17  | VAL  | HG21 | 0.990      | 0.05        | 2         |
| 1655     | A     | 17  | VAL  | HG22 | 0.990      | 0.05        | 2         |
| 1657     | A     | 17  | VAL  | HG23 | 0.990      | 0.05        | 2         |
| 1659     | A     | 17  | VAL  | C    | 175.975    | 0.3         | 1         |
| 1661     | A     | 17  | VAL  | CA   | 62.616     | 0.3         | 1         |
| 1663     | A     | 17  | VAL  | CB   | 32.841     | 0.3         | 1         |
| 1665     | A     | 17  | VAL  | CG1  | 22.008     | 0.3         | 2         |
| 1667     | A     | 17  | VAL  | CG2  | 21.976     | 0.3         | 2         |
| 1669     | A     | 17  | VAL  | N    | 125.650    | 0.3         | 1         |
| 1671     | A     | 18  | VAL  | H    | 9.187      | 0.05        | 1         |
| 1673     | A     | 18  | VAL  | HA   | 4.480      | 0.05        | 1         |
| 1675     | A     | 18  | VAL  | HB   | 1.949      | 0.05        | 1         |
| 1677     | A     | 18  | VAL  | HG11 | 0.926      | 0.05        | 2         |
| 1679     | A     | 18  | VAL  | HG12 | 0.926      | 0.05        | 2         |
| 1681     | A     | 18  | VAL  | HG13 | 0.926      | 0.05        | 2         |
| 1683     | A     | 18  | VAL  | HG21 | 0.985      | 0.05        | 2         |
| 1685     | A     | 18  | VAL  | HG22 | 0.985      | 0.05        | 2         |
| 1687     | A     | 18  | VAL  | HG23 | 0.985      | 0.05        | 2         |
| 1689     | A     | 18  | VAL  | C    | 174.240    | 0.3         | 1         |
| 1691     | A     | 18  | VAL  | CA   | 59.832     | 0.3         | 1         |
| 1693     | A     | 18  | VAL  | CB   | 34.369     | 0.3         | 1         |
| 1695     | A     | 18  | VAL  | CG1  | 20.135     | 0.3         | 2         |
| 1697     | A     | 18  | VAL  | CG2  | 21.961     | 0.3         | 2         |
| 1699     | A     | 18  | VAL  | N    | 127.579    | 0.3         | 1         |
| 1701     | A     | 19  | ARG  | H    | 8.173      | 0.05        | 1         |
| 1703     | A     | 19  | ARG  | HA   | 4.703      | 0.05        | 1         |
| 1705     | A     | 19  | ARG  | HB2  | 1.912      | 0.05        | 2         |
| 1707     | A     | 19  | ARG  | HB3  | 1.797      | 0.05        | 2         |
| 1709     | A     | 19  | ARG  | HD2  | 3.147      | 0.05        | 2         |
| 1711     | A     | 19  | ARG  | HG2  | 1.718      | 0.05        | 2         |
| 1713     | A     | 19  | ARG  | HG3  | 1.718      | 0.05        | 2         |
| 1715     | A     | 19  | ARG  | C    | 175.687    | 0.3         | 1         |
| 1717     | A     | 19  | ARG  | CA   | 54.233     | 0.3         | 1         |
| 1719     | A     | 19  | ARG  | CB   | 30.359     | 0.3         | 1         |
| 1721     | A     | 19  | ARG  | CD   | 43.500     | 0.3         | 1         |
| 1723     | A     | 19  | ARG  | CG   | 26.91      | 0.3         | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1725     | A     | 19  | ARG  | N    | 125.708    | 0.3         | 1         |
| 1727     | A     | 20  | LEU  | H    | 8.255      | 0.05        | 1         |
| 1729     | A     | 20  | LEU  | HB2  | 1.629      | 0.05        | 2         |
| 1731     | A     | 20  | LEU  | HB3  | 1.916      | 0.05        | 2         |
| 1733     | A     | 20  | LEU  | HD11 | 1.010      | 0.05        | 2         |
| 1735     | A     | 20  | LEU  | HD12 | 1.010      | 0.05        | 2         |
| 1737     | A     | 20  | LEU  | HD13 | 1.010      | 0.05        | 2         |
| 1739     | A     | 20  | LEU  | HD21 | 0.845      | 0.05        | 2         |
| 1741     | A     | 20  | LEU  | HD22 | 0.845      | 0.05        | 2         |
| 1743     | A     | 20  | LEU  | HD23 | 0.845      | 0.05        | 2         |
| 1745     | A     | 20  | LEU  | C    | 176.680    | 0.3         | 1         |
| 1747     | A     | 20  | LEU  | CA   | 52.960     | 0.3         | 1         |
| 1749     | A     | 20  | LEU  | CB   | 46.560     | 0.3         | 1         |
| 1751     | A     | 20  | LEU  | CD1  | 23.286     | 0.3         | 2         |
| 1753     | A     | 20  | LEU  | CD2  | 26.138     | 0.3         | 2         |
| 1755     | A     | 20  | LEU  | N    | 122.019    | 0.3         | 1         |
| 1757     | A     | 21  | TYR  | H    | 8.915      | 0.05        | 1         |
| 1759     | A     | 21  | TYR  | HA   | 4.65       | 0.05        | 1         |
| 1761     | A     | 21  | TYR  | HB2  | 3.406      | 0.05        | 2         |
| 1763     | A     | 21  | TYR  | HB3  | 2.604      | 0.05        | 2         |
| 1765     | A     | 21  | TYR  | HD1  | 7.432      | 0.05        | 3         |
| 1767     | A     | 21  | TYR  | HD2  | 7.432      | 0.05        | 3         |
| 1769     | A     | 21  | TYR  | HE1  | 6.82       | 0.05        | 3         |
| 1771     | A     | 21  | TYR  | HE2  | 6.82       | 0.05        | 3         |
| 1773     | A     | 21  | TYR  | CA   | 58.93      | 0.3         | 1         |
| 1775     | A     | 21  | TYR  | CB   | 37.2       | 0.3         | 1         |
| 1777     | A     | 21  | TYR  | CD1  | 133.4      | 0.3         | 3         |
| 1779     | A     | 21  | TYR  | CD2  | 133.4      | 0.3         | 3         |
| 1781     | A     | 21  | TYR  | CE1  | 118.3      | 0.3         | 3         |
| 1783     | A     | 21  | TYR  | CE2  | 118.3      | 0.3         | 3         |
| 1785     | A     | 21  | TYR  | N    | 120.637    | 0.3         | 1         |
| 1787     | A     | 22  | PRO  | HA   | 4.295      | 0.05        | 1         |
| 1789     | A     | 22  | PRO  | HB2  | 2.479      | 0.05        | 2         |
| 1791     | A     | 22  | PRO  | HB3  | 2.05       | 0.05        | 2         |
| 1793     | A     | 22  | PRO  | HD2  | 3.747      | 0.05        | 2         |
| 1795     | A     | 22  | PRO  | HD3  | 3.945      | 0.05        | 2         |
| 1797     | A     | 22  | PRO  | HG2  | 2.527      | 0.05        | 2         |
| 1799     | A     | 22  | PRO  | HG3  | 2.117      | 0.05        | 2         |
| 1801     | A     | 22  | PRO  | C    | 178.823    | 0.3         | 1         |
| 1803     | A     | 22  | PRO  | CA   | 67.002     | 0.3         | 1         |
| 1805     | A     | 22  | PRO  | CB   | 32.334     | 0.3         | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1807     | A     | 22  | PRO  | CD   | 51.15      | 0.3         | 1         |
| 1809     | A     | 22  | PRO  | CG   | 28.589     | 0.3         | 1         |
| 1811     | A     | 23  | ASP  | H    | 9.15       | 0.05        | 1         |
| 1813     | A     | 23  | ASP  | HA   | 4.50       | 0.05        | 1         |
| 1815     | A     | 23  | ASP  | HB2  | 2.86       | 0.05        | 2         |
| 1817     | A     | 23  | ASP  | HB3  | 2.723      | 0.05        | 2         |
| 1819     | A     | 23  | ASP  | C    | 179.364    | 0.3         | 1         |
| 1821     | A     | 23  | ASP  | CA   | 56.871     | 0.3         | 1         |
| 1823     | A     | 23  | ASP  | CB   | 39.34      | 0.3         | 1         |
| 1825     | A     | 23  | ASP  | N    | 114.907    | 0.3         | 1         |
| 1827     | A     | 24  | GLU  | H    | 7.515      | 0.05        | 1         |
| 1829     | A     | 24  | GLU  | HA   | 4.11       | 0.05        | 1         |
| 1831     | A     | 24  | GLU  | HB2  | 1.87       | 0.05        | 2         |
| 1833     | A     | 24  | GLU  | HB3  | 1.84       | 0.05        | 2         |
| 1835     | A     | 24  | GLU  | HG2  | 2.42       | 0.05        | 2         |
| 1837     | A     | 24  | GLU  | HG3  | 2.42       | 0.05        | 2         |
| 1839     | A     | 24  | GLU  | C    | 176.638    | 0.3         | 1         |
| 1841     | A     | 24  | GLU  | CA   | 58.5       | 0.3         | 1         |
| 1843     | A     | 24  | GLU  | CB   | 29.4       | 0.3         | 1         |
| 1845     | A     | 24  | GLU  | CG   | 36.88      | 0.3         | 1         |
| 1847     | A     | 24  | GLU  | N    | 123.513    | 0.3         | 1         |
| 1849     | A     | 25  | ILE  | H    | 7.85       | 0.05        | 1         |
| 1851     | A     | 25  | ILE  | HA   | 3.605      | 0.05        | 1         |
| 1853     | A     | 25  | ILE  | HB   | 2.071      | 0.05        | 1         |
| 1855     | A     | 25  | ILE  | HD11 | 0.85       | 0.05        | 1         |
| 1857     | A     | 25  | ILE  | HD12 | 0.85       | 0.05        | 1         |
| 1859     | A     | 25  | ILE  | HD13 | 0.85       | 0.05        | 1         |
| 1861     | A     | 25  | ILE  | HG12 | 1.796      | 0.05        | 2         |
| 1863     | A     | 25  | ILE  | HG13 | 0.859      | 0.05        | 2         |
| 1865     | A     | 25  | ILE  | HG21 | 0.98       | 0.05        | 1         |
| 1867     | A     | 25  | ILE  | HG22 | 0.98       | 0.05        | 1         |
| 1869     | A     | 25  | ILE  | HG23 | 0.98       | 0.05        | 1         |
| 1871     | A     | 25  | ILE  | C    | 178.317    | 0.3         | 1         |
| 1873     | A     | 25  | ILE  | CA   | 66.024     | 0.3         | 1         |
| 1875     | A     | 25  | ILE  | CB   | 37.613     | 0.3         | 1         |
| 1877     | A     | 25  | ILE  | CD1  | 13.64      | 0.3         | 1         |
| 1879     | A     | 25  | ILE  | CG1  | 30.95      | 0.3         | 1         |
| 1881     | A     | 25  | ILE  | CG2  | 17.32      | 0.3         | 1         |
| 1883     | A     | 25  | ILE  | N    | 119.2      | 0.3         | 1         |
| 1885     | A     | 26  | GLU  | H    | 8.07       | 0.05        | 1         |
| 1887     | A     | 26  | GLU  | HA   | 4.056      | 0.05        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1889     | A     | 26  | GLU  | HB2  | 2.165      | 0.05        | 2         |
| 1891     | A     | 26  | GLU  | HB3  | 2.167      | 0.05        | 2         |
| 1893     | A     | 26  | GLU  | HG2  | 2.457      | 0.05        | 2         |
| 1895     | A     | 26  | GLU  | HG3  | 2.457      | 0.05        | 2         |
| 1897     | A     | 26  | GLU  | C    | 179.616    | 0.3         | 1         |
| 1899     | A     | 26  | GLU  | CA   | 59.550     | 0.3         | 1         |
| 1901     | A     | 26  | GLU  | CB   | 29.411     | 0.3         | 1         |
| 1903     | A     | 26  | GLU  | CG   | 36.011     | 0.3         | 1         |
| 1905     | A     | 26  | GLU  | N    | 118.181    | 0.3         | 1         |
| 1907     | A     | 27  | ALA  | H    | 7.77       | 0.05        | 1         |
| 1909     | A     | 27  | ALA  | HA   | 4.26       | 0.05        | 1         |
| 1911     | A     | 27  | ALA  | HB1  | 1.656      | 0.05        | 1         |
| 1913     | A     | 27  | ALA  | HB2  | 1.656      | 0.05        | 1         |
| 1915     | A     | 27  | ALA  | HB3  | 1.656      | 0.05        | 1         |
| 1917     | A     | 27  | ALA  | CA   | 55.27      | 0.3         | 1         |
| 1919     | A     | 27  | ALA  | CB   | 18.527     | 0.3         | 1         |
| 1921     | A     | 27  | ALA  | N    | 121.839    | 0.3         | 1         |
| 1923     | A     | 28  | LEU  | H    | 8.39       | 0.05        | 1         |
| 1925     | A     | 28  | LEU  | HA   | 4.126      | 0.05        | 1         |
| 1927     | A     | 28  | LEU  | HB2  | 1.958      | 0.05        | 2         |
| 1929     | A     | 28  | LEU  | HB3  | 1.817      | 0.05        | 2         |
| 1931     | A     | 28  | LEU  | HD11 | 1.031      | 0.05        | 2         |
| 1933     | A     | 28  | LEU  | HD12 | 1.031      | 0.05        | 2         |
| 1935     | A     | 28  | LEU  | HD13 | 1.031      | 0.05        | 2         |
| 1937     | A     | 28  | LEU  | HD21 | 1.093      | 0.05        | 2         |
| 1939     | A     | 28  | LEU  | HD22 | 1.093      | 0.05        | 2         |
| 1941     | A     | 28  | LEU  | HD23 | 1.093      | 0.05        | 2         |
| 1943     | A     | 28  | LEU  | HG   | 1.771      | 0.05        | 1         |
| 1945     | A     | 28  | LEU  | C    | 179.223    | 0.3         | 1         |
| 1947     | A     | 28  | LEU  | CA   | 58.251     | 0.3         | 1         |
| 1949     | A     | 28  | LEU  | CB   | 42.454     | 0.3         | 1         |
| 1951     | A     | 28  | LEU  | CD1  | 25.302     | 0.3         | 1         |
| 1953     | A     | 28  | LEU  | CD2  | 24.676     | 0.3         | 1         |
| 1955     | A     | 28  | LEU  | CG   | 27.2       | 0.3         | 1         |
| 1957     | A     | 28  | LEU  | N    | 120.403    | 0.3         | 1         |
| 1959     | A     | 29  | LYS  | H    | 8.895      | 0.05        | 1         |
| 1961     | A     | 29  | LYS  | HA   | 3.858      | 0.05        | 1         |
| 1963     | A     | 29  | LYS  | HB2  | 1.994      | 0.05        | 2         |
| 1965     | A     | 29  | LYS  | HB3  | 1.994      | 0.05        | 2         |
| 1967     | A     | 29  | LYS  | HD2  | 1.785      | 0.05        | 2         |
| 1969     | A     | 29  | LYS  | HD3  | 1.745      | 0.05        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1971     | A     | 29  | LYS  | HE2  | 2.985      | 0.05        | 2         |
| 1973     | A     | 29  | LYS  | HE3  | 3.073      | 0.05        | 2         |
| 1975     | A     | 29  | LYS  | HG2  | 1.519      | 0.05        | 2         |
| 1977     | A     | 29  | LYS  | HG3  | 1.754      | 0.05        | 2         |
| 1979     | A     | 29  | LYS  | C    | 179.540    | 0.3         | 1         |
| 1981     | A     | 29  | LYS  | CA   | 60.333     | 0.3         | 1         |
| 1983     | A     | 29  | LYS  | CB   | 32.712     | 0.3         | 1         |
| 1985     | A     | 29  | LYS  | CD   | 29.875     | 0.3         | 1         |
| 1987     | A     | 29  | LYS  | CE   | 42.050     | 0.3         | 1         |
| 1989     | A     | 29  | LYS  | CG   | 26.135     | 0.3         | 1         |
| 1991     | A     | 29  | LYS  | N    | 118.430    | 0.3         | 1         |
| 1993     | A     | 30  | SER  | H    | 7.558      | 0.05        | 1         |
| 1995     | A     | 30  | SER  | HA   | 4.383      | 0.05        | 1         |
| 1997     | A     | 30  | SER  | HB2  | 4.110      | 0.05        | 2         |
| 1999     | A     | 30  | SER  | HB3  | 4.110      | 0.05        | 2         |
| 2001     | A     | 30  | SER  | CA   | 60.922     | 0.3         | 1         |
| 2003     | A     | 30  | SER  | CB   | 63.599     | 0.3         | 1         |
| 2005     | A     | 30  | SER  | N    | 111.985    | 0.3         | 1         |
| 2007     | A     | 31  | ARG  | H    | 7.763      | 0.05        | 1         |
| 2009     | A     | 31  | ARG  | HA   | 4.417      | 0.05        | 1         |
| 2011     | A     | 31  | ARG  | HB2  | 1.925      | 0.05        | 2         |
| 2013     | A     | 31  | ARG  | HB3  | 2.285      | 0.05        | 2         |
| 2015     | A     | 31  | ARG  | HD2  | 3.209      | 0.05        | 2         |
| 2017     | A     | 31  | ARG  | HD3  | 3.301      | 0.05        | 2         |
| 2019     | A     | 31  | ARG  | HG2  | 1.829      | 0.05        | 2         |
| 2021     | A     | 31  | ARG  | HG3  | 1.829      | 0.05        | 2         |
| 2023     | A     | 31  | ARG  | CA   | 55.41      | 0.3         | 1         |
| 2025     | A     | 31  | ARG  | CB   | 31.352     | 0.3         | 1         |
| 2027     | A     | 31  | ARG  | CD   | 43.052     | 0.3         | 1         |
| 2029     | A     | 31  | ARG  | CG   | 27.2       | 0.3         | 1         |
| 2031     | A     | 31  | ARG  | N    | 119.557    | 0.3         | 1         |
| 2033     | A     | 32  | VAL  | H    | 7.034      | 0.05        | 1         |
| 2035     | A     | 32  | VAL  | HA   | 3.280      | 0.05        | 1         |
| 2037     | A     | 32  | VAL  | HB   | 1.97       | 0.05        | 1         |
| 2039     | A     | 32  | VAL  | HG11 | 0.867      | 0.05        | 2         |
| 2041     | A     | 32  | VAL  | HG12 | 0.867      | 0.05        | 2         |
| 2043     | A     | 32  | VAL  | HG13 | 0.867      | 0.05        | 2         |
| 2045     | A     | 32  | VAL  | HG21 | 0.812      | 0.05        | 2         |
| 2047     | A     | 32  | VAL  | HG22 | 0.812      | 0.05        | 2         |
| 2049     | A     | 32  | VAL  | HG23 | 0.812      | 0.05        | 2         |
| 2051     | A     | 32  | VAL  | CA   | 61.133     | 0.3         | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 2053     | A     | 32  | VAL  | CB   | 32.467     | 0.3         | 1         |
| 2055     | A     | 32  | VAL  | CG1  | 21.79      | 0.3         | 2         |
| 2057     | A     | 32  | VAL  | CG2  | 22.01      | 0.3         | 2         |
| 2059     | A     | 32  | VAL  | N    | 121.674    | 0.3         | 1         |
| 2061     | A     | 33  | PRO  | HA   | 4.512      | 0.05        | 1         |
| 2063     | A     | 33  | PRO  | HB2  | 2.488      | 0.05        | 2         |
| 2065     | A     | 33  | PRO  | HB3  | 2.081      | 0.05        | 2         |
| 2067     | A     | 33  | PRO  | HD2  | 4.053      | 0.05        | 2         |
| 2069     | A     | 33  | PRO  | HD3  | 3.346      | 0.05        | 2         |
| 2071     | A     | 33  | PRO  | HG2  | 2.11       | 0.05        | 2         |
| 2073     | A     | 33  | PRO  | HG3  | 2.228      | 0.05        | 2         |
| 2075     | A     | 33  | PRO  | CA   | 62.841     | 0.3         | 1         |
| 2077     | A     | 33  | PRO  | CB   | 32.622     | 0.3         | 1         |
| 2079     | A     | 33  | PRO  | CD   | 51.690     | 0.3         | 1         |
| 2081     | A     | 33  | PRO  | CG   | 27.506     | 0.3         | 1         |
| 2083     | A     | 34  | ALA  | H    | 8.436      | 0.05        | 1         |
| 2085     | A     | 34  | ALA  | HA   | 4.227      | 0.05        | 1         |
| 2087     | A     | 34  | ALA  | HB1  | 1.490      | 0.05        | 1         |
| 2089     | A     | 34  | ALA  | HB2  | 1.490      | 0.05        | 1         |
| 2091     | A     | 34  | ALA  | HB3  | 1.490      | 0.05        | 1         |
| 2093     | A     | 34  | ALA  | C    | 179.218    | 0.3         | 1         |
| 2095     | A     | 34  | ALA  | CA   | 53.93      | 0.3         | 1         |
| 2097     | A     | 34  | ALA  | CB   | 18.533     | 0.3         | 1         |
| 2099     | A     | 34  | ALA  | N    | 121.917    | 0.3         | 1         |
| 2101     | A     | 35  | ASN  | H    | 8.684      | 0.05        | 1         |
| 2103     | A     | 35  | ASN  | HA   | 4.594      | 0.05        | 1         |
| 2105     | A     | 35  | ASN  | HB2  | 3.005      | 0.05        | 2         |
| 2107     | A     | 35  | ASN  | HB3  | 3.12       | 0.05        | 2         |
| 2109     | A     | 35  | ASN  | HD21 | 6.966      | 0.05        | 2         |
| 2111     | A     | 35  | ASN  | HD22 | 7.685      | 0.05        | 2         |
| 2113     | A     | 35  | ASN  | C    | 174.797    | 0.3         | 1         |
| 2115     | A     | 35  | ASN  | CA   | 54.245     | 0.3         | 1         |
| 2117     | A     | 35  | ASN  | CB   | 37.830     | 0.3         | 1         |
| 2119     | A     | 35  | ASN  | N    | 114.379    | 0.3         | 1         |
| 2121     | A     | 35  | ASN  | ND2  | 113.1      | 0.3         | 1         |
| 2123     | A     | 36  | THR  | H    | 7.730      | 0.05        | 1         |
| 2125     | A     | 36  | THR  | HA   | 4.635      | 0.05        | 1         |
| 2127     | A     | 36  | THR  | HB   | 4.121      | 0.05        | 1         |
| 2129     | A     | 36  | THR  | HG21 | 1.469      | 0.05        | 1         |
| 2131     | A     | 36  | THR  | HG22 | 1.469      | 0.05        | 1         |
| 2133     | A     | 36  | THR  | HG23 | 1.469      | 0.05        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 2135     | A     | 36  | THR  | CA   | 61.487     | 0.3         | 1         |
| 2137     | A     | 36  | THR  | CB   | 71.101     | 0.3         | 1         |
| 2139     | A     | 36  | THR  | CG2  | 20.573     | 0.3         | 1         |
| 2141     | A     | 36  | THR  | N    | 114.490    | 0.3         | 1         |
| 2143     | A     | 37  | SER  | H    | 8.622      | 0.05        | 1         |
| 2145     | A     | 37  | SER  | HA   | 4.664      | 0.05        | 1         |
| 2147     | A     | 37  | SER  | HB2  | 4.476      | 0.05        | 2         |
| 2149     | A     | 37  | SER  | HB3  | 4.141      | 0.05        | 2         |
| 2151     | A     | 37  | SER  | CA   | 56.974     | 0.3         | 1         |
| 2153     | A     | 37  | SER  | CB   | 65.755     | 0.3         | 1         |
| 2155     | A     | 37  | SER  | N    | 119.067    | 0.3         | 1         |
| 2157     | A     | 38  | MET  | H    | 9.125      | 0.05        | 1         |
| 2159     | A     | 38  | MET  | HA   | 4.235      | 0.05        | 1         |
| 2161     | A     | 38  | MET  | HB2  | 2.21       | 0.05        | 2         |
| 2163     | A     | 38  | MET  | HB3  | 2.589      | 0.05        | 2         |
| 2165     | A     | 38  | MET  | HE1  | 2.233      | 0.05        | 1         |
| 2167     | A     | 38  | MET  | HE2  | 2.233      | 0.05        | 1         |
| 2169     | A     | 38  | MET  | HE3  | 2.233      | 0.05        | 1         |
| 2171     | A     | 38  | MET  | C    | 178.508    | 0.3         | 1         |
| 2173     | A     | 38  | MET  | CA   | 59.967     | 0.3         | 1         |
| 2175     | A     | 38  | MET  | CB   | 32.376     | 0.3         | 1         |
| 2177     | A     | 38  | MET  | CE   | 16.866     | 0.3         | 1         |
| 2179     | A     | 38  | MET  | N    | 122.400    | 0.3         | 1         |
| 2181     | A     | 39  | SER  | H    | 8.626      | 0.05        | 1         |
| 2183     | A     | 39  | SER  | HA   | 4.18       | 0.05        | 1         |
| 2185     | A     | 39  | SER  | HB2  | 4.212      | 0.05        | 2         |
| 2187     | A     | 39  | SER  | HB3  | 4.076      | 0.05        | 2         |
| 2189     | A     | 39  | SER  | C    | 177.583    | 0.3         | 1         |
| 2191     | A     | 39  | SER  | CA   | 62.0       | 0.3         | 1         |
| 2193     | A     | 39  | SER  | CB   | 63.51      | 0.3         | 1         |
| 2195     | A     | 39  | SER  | N    | 112.404    | 0.3         | 1         |
| 2197     | A     | 40  | ALA  | H    | 8.134      | 0.05        | 1         |
| 2199     | A     | 40  | ALA  | HA   | 4.289      | 0.05        | 1         |
| 2201     | A     | 40  | ALA  | HB1  | 1.700      | 0.05        | 1         |
| 2203     | A     | 40  | ALA  | HB2  | 1.700      | 0.05        | 1         |
| 2205     | A     | 40  | ALA  | HB3  | 1.700      | 0.05        | 1         |
| 2207     | A     | 40  | ALA  | CA   | 55.240     | 0.3         | 1         |
| 2209     | A     | 40  | ALA  | CB   | 18.761     | 0.3         | 1         |
| 2211     | A     | 40  | ALA  | N    | 122.445    | 0.3         | 1         |
| 2213     | A     | 41  | TYR  | H    | 8.480      | 0.05        | 1         |
| 2215     | A     | 41  | TYR  | HA   | 4.29       | 0.05        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 2217     | A     | 41  | TYR  | HB2  | 3.251      | 0.05        | 2         |
| 2219     | A     | 41  | TYR  | HB3  | 3.250      | 0.05        | 2         |
| 2221     | A     | 41  | TYR  | HD1  | 6.99       | 0.05        | 3         |
| 2223     | A     | 41  | TYR  | HD2  | 6.99       | 0.05        | 3         |
| 2225     | A     | 41  | TYR  | HE1  | 6.798      | 0.05        | 3         |
| 2227     | A     | 41  | TYR  | HE2  | 6.798      | 0.05        | 3         |
| 2229     | A     | 41  | TYR  | C    | 177.802    | 0.3         | 1         |
| 2231     | A     | 41  | TYR  | CA   | 62.030     | 0.3         | 1         |
| 2233     | A     | 41  | TYR  | CB   | 39.893     | 0.3         | 1         |
| 2235     | A     | 41  | TYR  | CD1  | 132.7      | 0.3         | 3         |
| 2237     | A     | 41  | TYR  | CD2  | 132.7      | 0.3         | 3         |
| 2239     | A     | 41  | TYR  | CE1  | 119.0      | 0.3         | 3         |
| 2241     | A     | 41  | TYR  | CE2  | 119.0      | 0.3         | 3         |
| 2243     | A     | 41  | TYR  | N    | 121.110    | 0.3         | 1         |
| 2245     | A     | 42  | ILE  | H    | 8.726      | 0.05        | 1         |
| 2247     | A     | 42  | ILE  | HA   | 3.501      | 0.05        | 1         |
| 2249     | A     | 42  | ILE  | HB   | 1.950      | 0.05        | 1         |
| 2251     | A     | 42  | ILE  | HD11 | 0.803      | 0.05        | 1         |
| 2253     | A     | 42  | ILE  | HD12 | 0.803      | 0.05        | 1         |
| 2255     | A     | 42  | ILE  | HD13 | 0.803      | 0.05        | 1         |
| 2257     | A     | 42  | ILE  | HG12 | 2.227      | 0.05        | 2         |
| 2259     | A     | 42  | ILE  | HG13 | 0.808      | 0.05        | 2         |
| 2261     | A     | 42  | ILE  | HG21 | 0.875      | 0.05        | 1         |
| 2263     | A     | 42  | ILE  | HG22 | 0.875      | 0.05        | 1         |
| 2265     | A     | 42  | ILE  | HG23 | 0.875      | 0.05        | 1         |
| 2267     | A     | 42  | ILE  | C    | 178.148    | 0.3         | 1         |
| 2269     | A     | 42  | ILE  | CA   | 66.02      | 0.3         | 1         |
| 2271     | A     | 42  | ILE  | CB   | 37.624     | 0.3         | 1         |
| 2273     | A     | 42  | ILE  | CD1  | 14.07      | 0.3         | 1         |
| 2275     | A     | 42  | ILE  | CG1  | 29.985     | 0.3         | 1         |
| 2277     | A     | 42  | ILE  | CG2  | 18.327     | 0.3         | 1         |
| 2279     | A     | 42  | ILE  | N    | 118.174    | 0.3         | 1         |
| 2281     | A     | 43  | ARG  | H    | 8.52       | 0.05        | 1         |
| 2283     | A     | 43  | ARG  | HA   | 3.77       | 0.05        | 1         |
| 2285     | A     | 43  | ARG  | HB2  | 1.746      | 0.05        | 2         |
| 2287     | A     | 43  | ARG  | HB3  | 2.11       | 0.05        | 2         |
| 2289     | A     | 43  | ARG  | HG2  | 1.716      | 0.05        | 2         |
| 2291     | A     | 43  | ARG  | HG3  | 1.716      | 0.05        | 2         |
| 2293     | A     | 43  | ARG  | C    | 177.081    | 0.3         | 1         |
| 2295     | A     | 43  | ARG  | CA   | 60.97      | 0.3         | 1         |
| 2297     | A     | 43  | ARG  | CB   | 28.36      | 0.3         | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 2299     | A     | 43  | ARG  | CD   | 43.059     | 0.3         | 1         |
| 2301     | A     | 43  | ARG  | N    | 120.141    | 0.3         | 1         |
| 2303     | A     | 44  | ARG  | H    | 7.668      | 0.05        | 1         |
| 2305     | A     | 44  | ARG  | HA   | 3.956      | 0.05        | 1         |
| 2307     | A     | 44  | ARG  | HB2  | 2.06       | 0.05        | 2         |
| 2309     | A     | 44  | ARG  | HB3  | 1.98       | 0.05        | 2         |
| 2311     | A     | 44  | ARG  | HD2  | 3.245      | 0.05        | 2         |
| 2313     | A     | 44  | ARG  | HD3  | 3.35       | 0.05        | 2         |
| 2315     | A     | 44  | ARG  | HG2  | 1.762      | 0.05        | 2         |
| 2317     | A     | 44  | ARG  | HG3  | 1.762      | 0.05        | 2         |
| 2319     | A     | 44  | ARG  | C    | 178.607    | 0.3         | 1         |
| 2321     | A     | 44  | ARG  | CA   | 59.609     | 0.3         | 1         |
| 2323     | A     | 44  | ARG  | CB   | 29.760     | 0.3         | 1         |
| 2325     | A     | 44  | ARG  | CD   | 43.787     | 0.3         | 1         |
| 2327     | A     | 44  | ARG  | CG   | 26.530     | 0.3         | 1         |
| 2329     | A     | 44  | ARG  | N    | 118.718    | 0.3         | 1         |
| 2331     | A     | 45  | ILE  | H    | 7.693      | 0.05        | 1         |
| 2333     | A     | 45  | ILE  | HA   | 3.612      | 0.05        | 1         |
| 2335     | A     | 45  | ILE  | HB   | 1.884      | 0.05        | 1         |
| 2337     | A     | 45  | ILE  | HD11 | 0.388      | 0.05        | 1         |
| 2339     | A     | 45  | ILE  | HD12 | 0.388      | 0.05        | 1         |
| 2341     | A     | 45  | ILE  | HD13 | 0.388      | 0.05        | 1         |
| 2343     | A     | 45  | ILE  | HG12 | 1.156      | 0.05        | 2         |
| 2345     | A     | 45  | ILE  | HG13 | 0.398      | 0.05        | 2         |
| 2347     | A     | 45  | ILE  | HG21 | 0.576      | 0.05        | 1         |
| 2349     | A     | 45  | ILE  | HG22 | 0.576      | 0.05        | 1         |
| 2351     | A     | 45  | ILE  | HG23 | 0.576      | 0.05        | 1         |
| 2353     | A     | 45  | ILE  | C    | 175.056    | 0.3         | 1         |
| 2355     | A     | 45  | ILE  | CA   | 65.095     | 0.3         | 1         |
| 2357     | A     | 45  | ILE  | CB   | 37.634     | 0.3         | 1         |
| 2359     | A     | 45  | ILE  | CD1  | 13.836     | 0.3         | 1         |
| 2361     | A     | 45  | ILE  | CG1  | 27.38      | 0.3         | 1         |
| 2363     | A     | 45  | ILE  | CG2  | 17.699     | 0.3         | 1         |
| 2365     | A     | 45  | ILE  | N    | 118.487    | 0.3         | 1         |
| 2367     | A     | 46  | ILE  | H    | 8.405      | 0.05        | 1         |
| 2369     | A     | 46  | ILE  | HA   | 3.625      | 0.05        | 1         |
| 2371     | A     | 46  | ILE  | HB   | 2.196      | 0.05        | 1         |
| 2373     | A     | 46  | ILE  | HD11 | 0.925      | 0.05        | 1         |
| 2375     | A     | 46  | ILE  | HD12 | 0.925      | 0.05        | 1         |
| 2377     | A     | 46  | ILE  | HD13 | 0.925      | 0.05        | 1         |
| 2379     | A     | 46  | ILE  | HG12 | 1.943      | 0.05        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 2381     | A     | 46  | ILE  | HG13 | 0.931      | 0.05        | 2         |
| 2383     | A     | 46  | ILE  | HG21 | 0.993      | 0.05        | 1         |
| 2385     | A     | 46  | ILE  | HG22 | 0.993      | 0.05        | 1         |
| 2387     | A     | 46  | ILE  | HG23 | 0.993      | 0.05        | 1         |
| 2389     | A     | 46  | ILE  | C    | 178.004    | 0.3         | 1         |
| 2391     | A     | 46  | ILE  | CA   | 66.129     | 0.3         | 1         |
| 2393     | A     | 46  | ILE  | CB   | 38.012     | 0.3         | 1         |
| 2395     | A     | 46  | ILE  | CD1  | 15.948     | 0.3         | 1         |
| 2397     | A     | 46  | ILE  | CG1  | 29.426     | 0.3         | 1         |
| 2399     | A     | 46  | ILE  | CG2  | 17.660     | 0.3         | 1         |
| 2401     | A     | 46  | ILE  | N    | 122.0      | 0.3         | 1         |
| 2403     | A     | 47  | LEU  | H    | 8.935      | 0.05        | 1         |
| 2405     | A     | 47  | LEU  | HA   | 4.054      | 0.05        | 1         |
| 2407     | A     | 47  | LEU  | HB2  | 1.56       | 0.05        | 2         |
| 2409     | A     | 47  | LEU  | HB3  | 1.929      | 0.05        | 2         |
| 2411     | A     | 47  | LEU  | HD11 | 0.937      | 0.05        | 2         |
| 2413     | A     | 47  | LEU  | HD12 | 0.937      | 0.05        | 2         |
| 2415     | A     | 47  | LEU  | HD13 | 0.937      | 0.05        | 2         |
| 2417     | A     | 47  | LEU  | HD21 | 0.948      | 0.05        | 2         |
| 2419     | A     | 47  | LEU  | HD22 | 0.948      | 0.05        | 2         |
| 2421     | A     | 47  | LEU  | HD23 | 0.948      | 0.05        | 2         |
| 2423     | A     | 47  | LEU  | HG   | 2.009      | 0.05        | 1         |
| 2425     | A     | 47  | LEU  | C    | 180.461    | 0.3         | 1         |
| 2427     | A     | 47  | LEU  | CA   | 58.596     | 0.3         | 1         |
| 2429     | A     | 47  | LEU  | CB   | 40.633     | 0.3         | 1         |
| 2431     | A     | 47  | LEU  | CD1  | 24.895     | 0.3         | 2         |
| 2433     | A     | 47  | LEU  | CD2  | 21.560     | 0.3         | 2         |
| 2435     | A     | 47  | LEU  | CG   | 26.917     | 0.3         | 1         |
| 2437     | A     | 47  | LEU  | N    | 120.336    | 0.3         | 1         |
| 2439     | A     | 48  | ASN  | H    | 8.34       | 0.05        | 1         |
| 2441     | A     | 48  | ASN  | HA   | 4.524      | 0.05        | 1         |
| 2443     | A     | 48  | ASN  | HB2  | 2.912      | 0.05        | 2         |
| 2445     | A     | 48  | ASN  | HB3  | 2.95       | 0.05        | 2         |
| 2447     | A     | 48  | ASN  | HD21 | 6.915      | 0.05        | 2         |
| 2449     | A     | 48  | ASN  | HD22 | 7.787      | 0.05        | 2         |
| 2451     | A     | 48  | ASN  | C    | 178.720    | 0.3         | 1         |
| 2453     | A     | 48  | ASN  | CA   | 56.083     | 0.3         | 1         |
| 2455     | A     | 48  | ASN  | CB   | 38.129     | 0.3         | 1         |
| 2457     | A     | 48  | ASN  | N    | 117.516    | 0.3         | 1         |
| 2459     | A     | 48  | ASN  | ND2  | 111.00     | 0.3         | 1         |
| 2461     | A     | 49  | HIS  | H    | 7.85       | 0.05        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 2463     | A     | 49  | HIS  | HA   | 4.544      | 0.05        | 1         |
| 2465     | A     | 49  | HIS  | HB2  | 3.218      | 0.05        | 2         |
| 2467     | A     | 49  | HIS  | HB3  | 3.714      | 0.05        | 2         |
| 2469     | A     | 49  | HIS  | HD2  | 6.727      | 0.05        | 1         |
| 2471     | A     | 49  | HIS  | C    | 177.294    | 0.3         | 1         |
| 2473     | A     | 49  | HIS  | CA   | 59.101     | 0.3         | 1         |
| 2475     | A     | 49  | HIS  | CB   | 29.310     | 0.3         | 1         |
| 2477     | A     | 49  | HIS  | CD2  | 123.4      | 0.3         | 1         |
| 2479     | A     | 49  | HIS  | N    | 119.315    | 0.3         | 1         |
| 2481     | A     | 50  | LEU  | H    | 8.196      | 0.05        | 1         |
| 2483     | A     | 50  | LEU  | HA   | 4.055      | 0.05        | 1         |
| 2485     | A     | 50  | LEU  | HB2  | 1.617      | 0.05        | 2         |
| 2487     | A     | 50  | LEU  | HB3  | 2.069      | 0.05        | 2         |
| 2489     | A     | 50  | LEU  | HD11 | 0.89       | 0.05        | 2         |
| 2491     | A     | 50  | LEU  | HD12 | 0.89       | 0.05        | 2         |
| 2493     | A     | 50  | LEU  | HD13 | 0.89       | 0.05        | 2         |
| 2495     | A     | 50  | LEU  | HD21 | 1.000      | 0.05        | 2         |
| 2497     | A     | 50  | LEU  | HD22 | 1.000      | 0.05        | 2         |
| 2499     | A     | 50  | LEU  | HD23 | 1.000      | 0.05        | 2         |
| 2501     | A     | 50  | LEU  | C    | 178.471    | 0.3         | 1         |
| 2503     | A     | 50  | LEU  | CA   | 56.577     | 0.3         | 1         |
| 2505     | A     | 50  | LEU  | CB   | 42.060     | 0.3         | 1         |
| 2507     | A     | 50  | LEU  | CD1  | 22.47      | 0.3         | 2         |
| 2509     | A     | 50  | LEU  | CD2  | 25.659     | 0.3         | 2         |
| 2511     | A     | 50  | LEU  | N    | 117.173    | 0.3         | 1         |
| 2513     | A     | 51  | GLU  | H    | 7.75       | 0.05        | 1         |
| 2515     | A     | 51  | GLU  | HA   | 4.312      | 0.05        | 1         |
| 2517     | A     | 51  | GLU  | HB2  | 2.204      | 0.05        | 2         |
| 2519     | A     | 51  | GLU  | HB3  | 2.139      | 0.05        | 2         |
| 2521     | A     | 51  | GLU  | HG2  | 2.396      | 0.05        | 2         |
| 2523     | A     | 51  | GLU  | HG3  | 2.53       | 0.05        | 2         |
| 2525     | A     | 51  | GLU  | CA   | 57.23      | 0.3         | 1         |
| 2527     | A     | 51  | GLU  | CB   | 30.26      | 0.3         | 1         |
| 2529     | A     | 51  | GLU  | CG   | 36.32      | 0.3         | 1         |
| 2531     | A     | 51  | GLU  | N    | 117.196    | 0.3         | 1         |
| 2533     | A     | 52  | ASP  | H    | 7.827      | 0.05        | 1         |
| 2535     | A     | 52  | ASP  | HA   | 4.658      | 0.05        | 1         |
| 2537     | A     | 52  | ASP  | HB2  | 2.77       | 0.05        | 2         |
| 2539     | A     | 52  | ASP  | HB3  | 2.88       | 0.05        | 2         |
| 2541     | A     | 52  | ASP  | C    | 175.828    | 0.3         | 1         |
| 2543     | A     | 52  | ASP  | CA   | 54.871     | 0.3         | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 2545     | A     | 52  | ASP  | CB   | 41.57      | 0.3         | 1         |
| 2547     | A     | 52  | ASP  | N    | 120.128    | 0.3         | 1         |
| 2549     | A     | 53  | GLU  | H    | 7.919      | 0.05        | 1         |
| 2551     | A     | 53  | GLU  | HA   | 4.22       | 0.05        | 1         |
| 2553     | A     | 53  | GLU  | HB2  | 1.969      | 0.05        | 2         |
| 2555     | A     | 53  | GLU  | HB3  | 2.118      | 0.05        | 2         |
| 2557     | A     | 53  | GLU  | HG2  | 2.306      | 0.05        | 2         |
| 2559     | A     | 53  | GLU  | HG3  | 2.306      | 0.05        | 2         |
| 2561     | A     | 53  | GLU  | CA   | 58.02      | 0.3         | 1         |
| 2563     | A     | 53  | GLU  | CB   | 31.43      | 0.3         | 1         |
| 2565     | A     | 53  | GLU  | CG   | 36.72      | 0.3         | 1         |
| 2567     | A     | 53  | GLU  | N    | 125.725    | 0.3         | 1         |

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

- Residue not found in structure. All 642 occurrences are reported below.

| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 9   | GLY  | N    | 109.175    | 0.3         | 1         |
| B     | 51  | GLU  | HG2  | 2.396      | 0.05        | 2         |
| B     | 24  | GLU  | N    | 123.513    | 0.3         | 1         |
| B     | 33  | PRO  | CD   | 51.69      | 0.3         | 1         |
| B     | 17  | VAL  | HB   | 1.994      | 0.05        | 1         |
| B     | 33  | PRO  | HA   | 4.512      | 0.05        | 1         |
| B     | 40  | ALA  | N    | 122.445    | 0.3         | 1         |
| B     | 20  | LEU  | HD21 | 0.845      | 0.05        | 2         |
| B     | 26  | GLU  | CB   | 29.411     | 0.3         | 1         |
| B     | 18  | VAL  | CA   | 59.832     | 0.3         | 1         |
| B     | 17  | VAL  | C    | 175.975    | 0.3         | 1         |
| B     | 16  | VAL  | H    | 9.112      | 0.05        | 1         |
| B     | 5   | ARG  | H    | 8.522      | 0.05        | 1         |
| B     | 35  | ASN  | CA   | 54.245     | 0.3         | 1         |
| B     | 36  | THR  | N    | 114.49     | 0.3         | 1         |
| B     | 15  | PRO  | HD2  | 3.747      | 0.05        | 2         |
| B     | 6   | PRO  | HG2  | 2.05       | 0.05        | 2         |
| B     | 32  | VAL  | HG21 | 0.812      | 0.05        | 2         |
| B     | 14  | LYS  | CB   | 34.372     | 0.3         | 1         |
| B     | 29  | LYS  | CD   | 29.875     | 0.3         | 1         |
| B     | 32  | VAL  | HG13 | 0.867      | 0.05        | 2         |
| B     | 8   | GLY  | CA   | 45.46      | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 32  | VAL  | N    | 121.674    | 0.3         | 1         |
| B     | 46  | ILE  | HA   | 3.625      | 0.05        | 1         |
| B     | 11  | LYS  | HA   | 4.415      | 0.05        | 1         |
| B     | 15  | PRO  | HB3  | 1.932      | 0.05        | 2         |
| B     | 19  | ARG  | HG2  | 1.718      | 0.05        | 2         |
| B     | 46  | ILE  | CG2  | 17.66      | 0.3         | 1         |
| B     | 9   | GLY  | CA   | 45.5       | 0.3         | 1         |
| B     | 29  | LYS  | HG2  | 1.519      | 0.05        | 2         |
| B     | 26  | GLU  | H    | 8.07       | 0.05        | 1         |
| B     | 14  | LYS  | CE   | 42.416     | 0.3         | 1         |
| B     | 5   | ARG  | HB2  | 2.007      | 0.05        | 2         |
| B     | 4   | ARG  | HD3  | 3.224      | 0.05        | 2         |
| B     | 40  | ALA  | CA   | 55.24      | 0.3         | 1         |
| B     | 1   | MET  | HE2  | 2.166      | 0.05        | 1         |
| B     | 42  | ILE  | HG23 | 0.875      | 0.05        | 1         |
| B     | 30  | SER  | HA   | 4.383      | 0.05        | 1         |
| B     | 8   | GLY  | C    | 175.236    | 0.3         | 1         |
| B     | 45  | ILE  | HA   | 3.612      | 0.05        | 1         |
| B     | 25  | ILE  | HD13 | 0.85       | 0.05        | 1         |
| B     | 10  | LEU  | HG   | 1.712      | 0.05        | 1         |
| B     | 6   | PRO  | HD2  | 4.33       | 0.05        | 2         |
| B     | 29  | LYS  | HB2  | 1.994      | 0.05        | 2         |
| B     | 21  | TYR  | CE1  | 118.3      | 0.3         | 3         |
| B     | 23  | ASP  | HB2  | 2.86       | 0.05        | 2         |
| B     | 5   | ARG  | CD   | 43.676     | 0.3         | 1         |
| B     | 8   | GLY  | N    | 108.964    | 0.3         | 1         |
| B     | 17  | VAL  | HG23 | 0.99       | 0.05        | 2         |
| B     | 12  | ASP  | HB2  | 2.86       | 0.05        | 2         |
| B     | 11  | LYS  | N    | 119.917    | 0.3         | 1         |
| B     | 49  | HIS  | HB3  | 3.714      | 0.05        | 2         |
| B     | 31  | ARG  | HB3  | 2.285      | 0.05        | 2         |
| B     | 23  | ASP  | CB   | 39.34      | 0.3         | 1         |
| B     | 13  | THR  | HA   | 4.256      | 0.05        | 1         |
| B     | 16  | VAL  | C    | 174.696    | 0.3         | 1         |
| B     | 40  | ALA  | HB2  | 1.7        | 0.05        | 1         |
| B     | 10  | LEU  | HD21 | 0.907      | 0.05        | 2         |
| B     | 24  | GLU  | HB2  | 1.87       | 0.05        | 2         |
| B     | 25  | ILE  | HA   | 3.605      | 0.05        | 1         |
| B     | 3   | GLY  | HA3  | 4.05       | 0.05        | 2         |
| B     | 11  | LYS  | HB2  | 1.93       | 0.05        | 2         |
| B     | 30  | SER  | H    | 7.558      | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 11  | LYS  | HE2  | 3.08       | 0.05        | 2         |
| B     | 44  | ARG  | N    | 118.718    | 0.3         | 1         |
| B     | 19  | ARG  | N    | 125.708    | 0.3         | 1         |
| B     | 28  | LEU  | C    | 179.223    | 0.3         | 1         |
| B     | 31  | ARG  | CD   | 43.052     | 0.3         | 1         |
| B     | 1   | MET  | HG3  | 2.61       | 0.05        | 2         |
| B     | 12  | ASP  | CA   | 54.4       | 0.3         | 1         |
| B     | 47  | LEU  | CG   | 26.917     | 0.3         | 1         |
| B     | 33  | PRO  | HB2  | 2.488      | 0.05        | 2         |
| B     | 44  | ARG  | HD3  | 3.35       | 0.05        | 2         |
| B     | 52  | ASP  | HA   | 4.658      | 0.05        | 1         |
| B     | 14  | LYS  | HB2  | 1.909      | 0.05        | 2         |
| B     | 6   | PRO  | HB3  | 2.408      | 0.05        | 2         |
| B     | 42  | ILE  | HB   | 1.95       | 0.05        | 1         |
| B     | 10  | LEU  | HD12 | 0.98       | 0.05        | 2         |
| B     | 24  | GLU  | H    | 7.515      | 0.05        | 1         |
| B     | 47  | LEU  | H    | 8.935      | 0.05        | 1         |
| B     | 35  | ASN  | ND2  | 113.1      | 0.3         | 1         |
| B     | 11  | LYS  | HG3  | 1.55       | 0.05        | 2         |
| B     | 50  | LEU  | CA   | 56.577     | 0.3         | 1         |
| B     | 30  | SER  | HB2  | 4.11       | 0.05        | 2         |
| B     | 30  | SER  | CB   | 63.599     | 0.3         | 1         |
| B     | 39  | SER  | N    | 112.404    | 0.3         | 1         |
| B     | 51  | GLU  | N    | 117.196    | 0.3         | 1         |
| B     | 9   | GLY  | HA3  | 4.03       | 0.05        | 2         |
| B     | 20  | LEU  | HD22 | 0.845      | 0.05        | 2         |
| B     | 26  | GLU  | CA   | 59.55      | 0.3         | 1         |
| B     | 4   | ARG  | N    | 120.49     | 0.3         | 1         |
| B     | 18  | VAL  | HA   | 4.48       | 0.05        | 1         |
| B     | 46  | ILE  | HD12 | 0.925      | 0.05        | 1         |
| B     | 21  | TYR  | HD2  | 7.432      | 0.05        | 3         |
| B     | 49  | HIS  | H    | 7.85       | 0.05        | 1         |
| B     | 44  | ARG  | HD2  | 3.245      | 0.05        | 2         |
| B     | 20  | LEU  | HD12 | 1.01       | 0.05        | 2         |
| B     | 16  | VAL  | HG23 | 0.865      | 0.05        | 2         |
| B     | 52  | ASP  | N    | 120.128    | 0.3         | 1         |
| B     | 12  | ASP  | N    | 118.931    | 0.3         | 1         |
| B     | 39  | SER  | HB2  | 4.212      | 0.05        | 2         |
| B     | 4   | ARG  | HG2  | 1.665      | 0.05        | 2         |
| B     | 15  | PRO  | CG   | 26.933     | 0.3         | 1         |
| B     | 4   | ARG  | CA   | 55.82      | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 31  | ARG  | HG3  | 1.829      | 0.05        | 2         |
| B     | 8   | GLY  | HA2  | 4.07       | 0.05        | 2         |
| B     | 33  | PRO  | HG2  | 2.11       | 0.05        | 2         |
| B     | 50  | LEU  | N    | 117.173    | 0.3         | 1         |
| B     | 11  | LYS  | HD2  | 1.778      | 0.05        | 2         |
| B     | 25  | ILE  | CB   | 37.613     | 0.3         | 1         |
| B     | 51  | GLU  | CA   | 57.23      | 0.3         | 1         |
| B     | 41  | TYR  | HD1  | 6.99       | 0.05        | 3         |
| B     | 32  | VAL  | CG2  | 22.01      | 0.3         | 2         |
| B     | 7   | GLY  | CA   | 45.26      | 0.3         | 1         |
| B     | 48  | ASN  | C    | 178.72     | 0.3         | 1         |
| B     | 44  | ARG  | CB   | 29.76      | 0.3         | 1         |
| B     | 52  | ASP  | C    | 175.828    | 0.3         | 1         |
| B     | 50  | LEU  | HD22 | 1.0        | 0.05        | 2         |
| B     | 53  | GLU  | HG2  | 2.306      | 0.05        | 2         |
| B     | 14  | LYS  | HA   | 4.952      | 0.05        | 1         |
| B     | 46  | ILE  | C    | 178.004    | 0.3         | 1         |
| B     | 17  | VAL  | H    | 8.338      | 0.05        | 1         |
| B     | 39  | SER  | C    | 177.583    | 0.3         | 1         |
| B     | 27  | ALA  | HB3  | 1.656      | 0.05        | 1         |
| B     | 10  | LEU  | HB3  | 1.647      | 0.05        | 2         |
| B     | 22  | PRO  | HA   | 4.295      | 0.05        | 1         |
| B     | 6   | PRO  | HA   | 4.55       | 0.05        | 1         |
| B     | 2   | VAL  | HG23 | 1.037      | 0.05        | 2         |
| B     | 14  | LYS  | HD2  | 1.78       | 0.05        | 2         |
| B     | 10  | LEU  | N    | 121.467    | 0.3         | 1         |
| B     | 40  | ALA  | HB1  | 1.7        | 0.05        | 1         |
| B     | 46  | ILE  | HG13 | 0.931      | 0.05        | 2         |
| B     | 41  | TYR  | HE2  | 6.798      | 0.05        | 3         |
| B     | 14  | LYS  | CA   | 52.486     | 0.3         | 1         |
| B     | 30  | SER  | N    | 111.985    | 0.3         | 1         |
| B     | 46  | ILE  | CD1  | 15.948     | 0.3         | 1         |
| B     | 45  | ILE  | HD13 | 0.388      | 0.05        | 1         |
| B     | 47  | LEU  | C    | 180.461    | 0.3         | 1         |
| B     | 21  | TYR  | CE2  | 118.3      | 0.3         | 3         |
| B     | 36  | THR  | CA   | 61.487     | 0.3         | 1         |
| B     | 43  | ARG  | HG2  | 1.716      | 0.05        | 2         |
| B     | 45  | ILE  | HG21 | 0.576      | 0.05        | 1         |
| B     | 2   | VAL  | CG2  | 21.0       | 0.3         | 2         |
| B     | 40  | ALA  | H    | 8.134      | 0.05        | 1         |
| B     | 28  | LEU  | HB2  | 1.958      | 0.05        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 31  | ARG  | CG   | 27.2       | 0.3         | 1         |
| B     | 15  | PRO  | HD3  | 3.861      | 0.05        | 2         |
| B     | 4   | ARG  | CD   | 43.419     | 0.3         | 1         |
| B     | 12  | ASP  | CB   | 41.82      | 0.3         | 1         |
| B     | 15  | PRO  | CB   | 33.036     | 0.3         | 1         |
| B     | 41  | TYR  | HB2  | 3.251      | 0.05        | 2         |
| B     | 2   | VAL  | HG12 | 1.037      | 0.05        | 2         |
| B     | 41  | TYR  | CA   | 62.03      | 0.3         | 1         |
| B     | 47  | LEU  | HD23 | 0.948      | 0.05        | 2         |
| B     | 44  | ARG  | HB2  | 2.06       | 0.05        | 2         |
| B     | 42  | ILE  | HG12 | 2.227      | 0.05        | 2         |
| B     | 13  | THR  | HG22 | 0.317      | 0.05        | 1         |
| B     | 47  | LEU  | HA   | 4.054      | 0.05        | 1         |
| B     | 29  | LYS  | H    | 8.895      | 0.05        | 1         |
| B     | 20  | LEU  | HB3  | 1.916      | 0.05        | 2         |
| B     | 42  | ILE  | H    | 8.726      | 0.05        | 1         |
| B     | 41  | TYR  | CB   | 39.893     | 0.3         | 1         |
| B     | 49  | HIS  | HA   | 4.544      | 0.05        | 1         |
| B     | 32  | VAL  | HA   | 3.28       | 0.05        | 1         |
| B     | 53  | GLU  | HB2  | 1.969      | 0.05        | 2         |
| B     | 50  | LEU  | CB   | 42.06      | 0.3         | 1         |
| B     | 14  | LYS  | N    | 119.891    | 0.3         | 1         |
| B     | 14  | LYS  | HE3  | 3.059      | 0.05        | 2         |
| B     | 46  | ILE  | HG23 | 0.993      | 0.05        | 1         |
| B     | 50  | LEU  | HA   | 4.055      | 0.05        | 1         |
| B     | 46  | ILE  | HD11 | 0.925      | 0.05        | 1         |
| B     | 21  | TYR  | HD1  | 7.432      | 0.05        | 3         |
| B     | 43  | ARG  | CA   | 60.97      | 0.3         | 1         |
| B     | 13  | THR  | N    | 107.789    | 0.3         | 1         |
| B     | 36  | THR  | H    | 7.73       | 0.05        | 1         |
| B     | 38  | MET  | HE2  | 2.233      | 0.05        | 1         |
| B     | 40  | ALA  | HB3  | 1.7        | 0.05        | 1         |
| B     | 22  | PRO  | C    | 178.823    | 0.3         | 1         |
| B     | 32  | VAL  | CB   | 32.467     | 0.3         | 1         |
| B     | 16  | VAL  | HA   | 4.29       | 0.05        | 1         |
| B     | 1   | MET  | CG   | 32.138     | 0.3         | 1         |
| B     | 9   | GLY  | H    | 8.533      | 0.05        | 1         |
| B     | 41  | TYR  | C    | 177.802    | 0.3         | 1         |
| B     | 11  | LYS  | CE   | 42.421     | 0.3         | 1         |
| B     | 41  | TYR  | HD2  | 6.99       | 0.05        | 3         |
| B     | 1   | MET  | C    | 176.534    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 21  | TYR  | HB3  | 2.604      | 0.05        | 2         |
| B     | 36  | THR  | CG2  | 20.573     | 0.3         | 1         |
| B     | 18  | VAL  | CG2  | 21.961     | 0.3         | 2         |
| B     | 17  | VAL  | HG12 | 0.83       | 0.05        | 2         |
| B     | 7   | GLY  | HA3  | 4.09       | 0.05        | 2         |
| B     | 12  | ASP  | HA   | 4.85       | 0.05        | 1         |
| B     | 13  | THR  | CG2  | 20.656     | 0.3         | 1         |
| B     | 49  | HIS  | C    | 177.294    | 0.3         | 1         |
| B     | 51  | GLU  | HG3  | 2.53       | 0.05        | 2         |
| B     | 29  | LYS  | HD2  | 1.785      | 0.05        | 2         |
| B     | 47  | LEU  | HB2  | 1.56       | 0.05        | 2         |
| B     | 17  | VAL  | HA   | 4.496      | 0.05        | 1         |
| B     | 34  | ALA  | HB1  | 1.49       | 0.05        | 1         |
| B     | 20  | LEU  | CB   | 46.56      | 0.3         | 1         |
| B     | 43  | ARG  | N    | 120.141    | 0.3         | 1         |
| B     | 28  | LEU  | HD12 | 1.031      | 0.05        | 2         |
| B     | 47  | LEU  | HD11 | 0.937      | 0.05        | 2         |
| B     | 5   | ARG  | HD2  | 3.354      | 0.05        | 2         |
| B     | 6   | PRO  | HG3  | 2.05       | 0.05        | 2         |
| B     | 29  | LYS  | CE   | 42.05      | 0.3         | 1         |
| B     | 10  | LEU  | HD11 | 0.98       | 0.05        | 2         |
| B     | 18  | VAL  | HG11 | 0.926      | 0.05        | 2         |
| B     | 3   | GLY  | N    | 112.524    | 0.3         | 1         |
| B     | 37  | SER  | HA   | 4.664      | 0.05        | 1         |
| B     | 46  | ILE  | HB   | 2.196      | 0.05        | 1         |
| B     | 11  | LYS  | CB   | 32.929     | 0.3         | 1         |
| B     | 18  | VAL  | HG23 | 0.985      | 0.05        | 2         |
| B     | 19  | ARG  | HG3  | 1.718      | 0.05        | 2         |
| B     | 23  | ASP  | N    | 114.907    | 0.3         | 1         |
| B     | 46  | ILE  | CG1  | 29.426     | 0.3         | 1         |
| B     | 20  | LEU  | H    | 8.255      | 0.05        | 1         |
| B     | 11  | LYS  | HE3  | 3.08       | 0.05        | 2         |
| B     | 24  | GLU  | HG2  | 2.42       | 0.05        | 2         |
| B     | 1   | MET  | HE3  | 2.166      | 0.05        | 1         |
| B     | 42  | ILE  | HG22 | 0.875      | 0.05        | 1         |
| B     | 18  | VAL  | HG12 | 0.926      | 0.05        | 2         |
| B     | 36  | THR  | CB   | 71.101     | 0.3         | 1         |
| B     | 39  | SER  | H    | 8.626      | 0.05        | 1         |
| B     | 2   | VAL  | CG1  | 21.0       | 0.3         | 2         |
| B     | 19  | ARG  | CB   | 30.359     | 0.3         | 1         |
| B     | 24  | GLU  | C    | 176.638    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 38  | MET  | HB2  | 2.21       | 0.05        | 2         |
| B     | 38  | MET  | C    | 178.508    | 0.3         | 1         |
| B     | 29  | LYS  | HB3  | 1.994      | 0.05        | 2         |
| B     | 36  | THR  | HG21 | 1.469      | 0.05        | 1         |
| B     | 1   | MET  | HA   | 4.562      | 0.05        | 1         |
| B     | 23  | ASP  | HB3  | 2.723      | 0.05        | 2         |
| B     | 5   | ARG  | CG   | 26.489     | 0.3         | 1         |
| B     | 49  | HIS  | N    | 119.315    | 0.3         | 1         |
| B     | 12  | ASP  | HB3  | 3.01       | 0.05        | 2         |
| B     | 12  | ASP  | C    | 176.436    | 0.3         | 1         |
| B     | 52  | ASP  | H    | 7.827      | 0.05        | 1         |
| B     | 44  | ARG  | HG2  | 1.762      | 0.05        | 2         |
| B     | 22  | PRO  | HG3  | 2.117      | 0.05        | 2         |
| B     | 31  | ARG  | HB2  | 1.925      | 0.05        | 2         |
| B     | 13  | THR  | HB   | 3.681      | 0.05        | 1         |
| B     | 26  | GLU  | HG2  | 2.457      | 0.05        | 2         |
| B     | 24  | GLU  | CA   | 58.5       | 0.3         | 1         |
| B     | 20  | LEU  | CD1  | 23.286     | 0.3         | 2         |
| B     | 39  | SER  | CB   | 63.51      | 0.3         | 1         |
| B     | 19  | ARG  | H    | 8.173      | 0.05        | 1         |
| B     | 45  | ILE  | HB   | 1.884      | 0.05        | 1         |
| B     | 50  | LEU  | HD23 | 1.0        | 0.05        | 2         |
| B     | 15  | PRO  | HG3  | 2.13       | 0.05        | 2         |
| B     | 43  | ARG  | HB2  | 1.746      | 0.05        | 2         |
| B     | 45  | ILE  | CA   | 65.095     | 0.3         | 1         |
| B     | 48  | ASN  | ND2  | 111.0      | 0.3         | 1         |
| B     | 33  | PRO  | HB3  | 2.081      | 0.05        | 2         |
| B     | 32  | VAL  | CA   | 61.133     | 0.3         | 1         |
| B     | 16  | VAL  | HG11 | 0.902      | 0.05        | 2         |
| B     | 16  | VAL  | HB   | 2.054      | 0.05        | 1         |
| B     | 53  | GLU  | CG   | 36.72      | 0.3         | 1         |
| B     | 14  | LYS  | HB3  | 1.657      | 0.05        | 2         |
| B     | 6   | PRO  | CB   | 32.259     | 0.3         | 1         |
| B     | 6   | PRO  | HB2  | 2.054      | 0.05        | 2         |
| B     | 10  | LEU  | HD13 | 0.98       | 0.05        | 2         |
| B     | 47  | LEU  | CD1  | 24.895     | 0.3         | 2         |
| B     | 28  | LEU  | HD21 | 1.093      | 0.05        | 2         |
| B     | 34  | ALA  | H    | 8.436      | 0.05        | 1         |
| B     | 17  | VAL  | HG11 | 0.83       | 0.05        | 2         |
| B     | 22  | PRO  | HD2  | 3.747      | 0.05        | 2         |
| B     | 10  | LEU  | CG   | 27.117     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 45  | ILE  | CD1  | 13.836     | 0.3         | 1         |
| B     | 37  | SER  | H    | 8.622      | 0.05        | 1         |
| B     | 49  | HIS  | CD2  | 123.4      | 0.3         | 1         |
| B     | 18  | VAL  | H    | 9.187      | 0.05        | 1         |
| B     | 30  | SER  | HB3  | 4.11       | 0.05        | 2         |
| B     | 45  | ILE  | HG13 | 0.398      | 0.05        | 2         |
| B     | 10  | LEU  | CD2  | 23.3       | 0.3         | 2         |
| B     | 4   | ARG  | H    | 8.159      | 0.05        | 1         |
| B     | 20  | LEU  | HD23 | 0.845      | 0.05        | 2         |
| B     | 26  | GLU  | HB3  | 2.167      | 0.05        | 2         |
| B     | 28  | LEU  | CG   | 27.2       | 0.3         | 1         |
| B     | 37  | SER  | HB3  | 4.141      | 0.05        | 2         |
| B     | 18  | VAL  | HB   | 1.949      | 0.05        | 1         |
| B     | 49  | HIS  | HD2  | 6.727      | 0.05        | 1         |
| B     | 47  | LEU  | HD12 | 0.937      | 0.05        | 2         |
| B     | 50  | LEU  | C    | 178.471    | 0.3         | 1         |
| B     | 1   | MET  | CB   | 33.026     | 0.3         | 1         |
| B     | 45  | ILE  | N    | 118.487    | 0.3         | 1         |
| B     | 32  | VAL  | HG23 | 0.812      | 0.05        | 2         |
| B     | 20  | LEU  | HD11 | 1.01       | 0.05        | 2         |
| B     | 16  | VAL  | HG22 | 0.865      | 0.05        | 2         |
| B     | 4   | ARG  | HB2  | 1.9        | 0.05        | 2         |
| B     | 26  | GLU  | C    | 179.616    | 0.3         | 1         |
| B     | 38  | MET  | CE   | 16.866     | 0.3         | 1         |
| B     | 22  | PRO  | CG   | 28.589     | 0.3         | 1         |
| B     | 19  | ARG  | HB3  | 1.797      | 0.05        | 2         |
| B     | 37  | SER  | CB   | 65.755     | 0.3         | 1         |
| B     | 11  | LYS  | CA   | 57.22      | 0.3         | 1         |
| B     | 42  | ILE  | HD13 | 0.803      | 0.05        | 1         |
| B     | 45  | ILE  | CG1  | 27.38      | 0.3         | 1         |
| B     | 33  | PRO  | HD2  | 4.053      | 0.05        | 2         |
| B     | 4   | ARG  | CB   | 31.179     | 0.3         | 1         |
| B     | 33  | PRO  | CA   | 62.841     | 0.3         | 1         |
| B     | 43  | ARG  | HA   | 3.77       | 0.05        | 1         |
| B     | 51  | GLU  | H    | 7.75       | 0.05        | 1         |
| B     | 50  | LEU  | HD11 | 0.89       | 0.05        | 2         |
| B     | 32  | VAL  | CG1  | 21.79      | 0.3         | 2         |
| B     | 25  | ILE  | HD11 | 0.85       | 0.05        | 1         |
| B     | 48  | ASN  | CB   | 38.129     | 0.3         | 1         |
| B     | 10  | LEU  | HA   | 4.312      | 0.05        | 1         |
| B     | 44  | ARG  | CA   | 59.609     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 19  | ARG  | CA   | 54.233     | 0.3         | 1         |
| B     | 46  | ILE  | CB   | 38.012     | 0.3         | 1         |
| B     | 50  | LEU  | HD21 | 1.0        | 0.05        | 2         |
| B     | 53  | GLU  | HG3  | 2.306      | 0.05        | 2         |
| B     | 29  | LYS  | CA   | 60.333     | 0.3         | 1         |
| B     | 16  | VAL  | CB   | 34.265     | 0.3         | 1         |
| B     | 5   | ARG  | CB   | 29.728     | 0.3         | 1         |
| B     | 31  | ARG  | HD3  | 3.301      | 0.05        | 2         |
| B     | 31  | ARG  | HA   | 4.417      | 0.05        | 1         |
| B     | 17  | VAL  | HG21 | 0.99       | 0.05        | 2         |
| B     | 45  | ILE  | H    | 7.693      | 0.05        | 1         |
| B     | 25  | ILE  | HG21 | 0.98       | 0.05        | 1         |
| B     | 48  | ASN  | HD21 | 6.915      | 0.05        | 2         |
| B     | 2   | VAL  | HG22 | 1.037      | 0.05        | 2         |
| B     | 44  | ARG  | HA   | 3.956      | 0.05        | 1         |
| B     | 19  | ARG  | HA   | 4.703      | 0.05        | 1         |
| B     | 41  | TYR  | N    | 121.11     | 0.3         | 1         |
| B     | 17  | VAL  | CG1  | 22.008     | 0.3         | 2         |
| B     | 14  | LYS  | HD3  | 1.775      | 0.05        | 2         |
| B     | 10  | LEU  | HD23 | 0.907      | 0.05        | 2         |
| B     | 48  | ASN  | H    | 8.34       | 0.05        | 1         |
| B     | 1   | MET  | HB3  | 2.147      | 0.05        | 2         |
| B     | 39  | SER  | CA   | 62.0       | 0.3         | 1         |
| B     | 40  | ALA  | HA   | 4.289      | 0.05        | 1         |
| B     | 21  | TYR  | HE1  | 6.82       | 0.05        | 3         |
| B     | 46  | ILE  | H    | 8.405      | 0.05        | 1         |
| B     | 42  | ILE  | CD1  | 14.07      | 0.3         | 1         |
| B     | 24  | GLU  | CB   | 29.4       | 0.3         | 1         |
| B     | 21  | TYR  | CB   | 37.2       | 0.3         | 1         |
| B     | 45  | ILE  | HG22 | 0.576      | 0.05        | 1         |
| B     | 26  | GLU  | HA   | 4.056      | 0.05        | 1         |
| B     | 45  | ILE  | C    | 175.056    | 0.3         | 1         |
| B     | 29  | LYS  | HE3  | 3.073      | 0.05        | 2         |
| B     | 13  | THR  | CB   | 72.453     | 0.3         | 1         |
| B     | 36  | THR  | HG22 | 1.469      | 0.05        | 1         |
| B     | 45  | ILE  | CB   | 37.634     | 0.3         | 1         |
| B     | 43  | ARG  | C    | 177.081    | 0.3         | 1         |
| B     | 29  | LYS  | N    | 118.43     | 0.3         | 1         |
| B     | 24  | GLU  | HA   | 4.11       | 0.05        | 1         |
| B     | 42  | ILE  | N    | 118.174    | 0.3         | 1         |
| B     | 7   | GLY  | H    | 8.615      | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 47  | LEU  | CA   | 58.596     | 0.3         | 1         |
| B     | 2   | VAL  | HG13 | 1.037      | 0.05        | 2         |
| B     | 53  | GLU  | CB   | 31.43      | 0.3         | 1         |
| B     | 23  | ASP  | HA   | 4.5        | 0.05        | 1         |
| B     | 15  | PRO  | C    | 177.155    | 0.3         | 1         |
| B     | 47  | LEU  | HD22 | 0.948      | 0.05        | 2         |
| B     | 42  | ILE  | HG13 | 0.808      | 0.05        | 2         |
| B     | 13  | THR  | HG21 | 0.317      | 0.05        | 1         |
| B     | 20  | LEU  | HB2  | 1.629      | 0.05        | 2         |
| B     | 28  | LEU  | HD22 | 1.093      | 0.05        | 2         |
| B     | 2   | VAL  | N    | 121.358    | 0.3         | 1         |
| B     | 32  | VAL  | HB   | 1.97       | 0.05        | 1         |
| B     | 21  | TYR  | H    | 8.915      | 0.05        | 1         |
| B     | 14  | LYS  | HE2  | 3.119      | 0.05        | 2         |
| B     | 23  | ASP  | H    | 9.15       | 0.05        | 1         |
| B     | 10  | LEU  | CD1  | 25.09      | 0.3         | 2         |
| B     | 46  | ILE  | HG22 | 0.993      | 0.05        | 1         |
| B     | 26  | GLU  | CG   | 36.011     | 0.3         | 1         |
| B     | 28  | LEU  | CB   | 42.454     | 0.3         | 1         |
| B     | 28  | LEU  | HG   | 1.771      | 0.05        | 1         |
| B     | 27  | ALA  | CA   | 55.27      | 0.3         | 1         |
| B     | 28  | LEU  | HD13 | 1.031      | 0.05        | 2         |
| B     | 2   | VAL  | H    | 8.215      | 0.05        | 1         |
| B     | 48  | ASN  | N    | 117.516    | 0.3         | 1         |
| B     | 20  | LEU  | N    | 122.019    | 0.3         | 1         |
| B     | 43  | ARG  | CB   | 28.36      | 0.3         | 1         |
| B     | 53  | GLU  | H    | 7.919      | 0.05        | 1         |
| B     | 38  | MET  | HE1  | 2.233      | 0.05        | 1         |
| B     | 50  | LEU  | HD12 | 0.89       | 0.05        | 2         |
| B     | 9   | GLY  | HA2  | 4.03       | 0.05        | 2         |
| B     | 16  | VAL  | HG21 | 0.865      | 0.05        | 2         |
| B     | 46  | ILE  | N    | 122.0      | 0.3         | 1         |
| B     | 5   | ARG  | N    | 123.728    | 0.3         | 1         |
| B     | 11  | LYS  | CD   | 29.35      | 0.3         | 1         |
| B     | 21  | TYR  | HB2  | 3.406      | 0.05        | 2         |
| B     | 18  | VAL  | CG1  | 20.135     | 0.3         | 2         |
| B     | 4   | ARG  | CG   | 27.15      | 0.3         | 1         |
| B     | 28  | LEU  | H    | 8.39       | 0.05        | 1         |
| B     | 21  | TYR  | CD1  | 133.4      | 0.3         | 3         |
| B     | 43  | ARG  | H    | 8.52       | 0.05        | 1         |
| B     | 29  | LYS  | HD3  | 1.745      | 0.05        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 47  | LEU  | HB3  | 1.929      | 0.05        | 2         |
| B     | 7   | GLY  | C    | 175.353    | 0.3         | 1         |
| B     | 48  | ASN  | CA   | 56.083     | 0.3         | 1         |
| B     | 34  | ALA  | HB2  | 1.49       | 0.05        | 1         |
| B     | 20  | LEU  | CA   | 52.96      | 0.3         | 1         |
| B     | 21  | TYR  | N    | 120.637    | 0.3         | 1         |
| B     | 44  | ARG  | CD   | 43.787     | 0.3         | 1         |
| B     | 22  | PRO  | HB2  | 2.479      | 0.05        | 2         |
| B     | 18  | VAL  | C    | 174.24     | 0.3         | 1         |
| B     | 19  | ARG  | CD   | 43.5       | 0.3         | 1         |
| B     | 17  | VAL  | CA   | 62.616     | 0.3         | 1         |
| B     | 46  | ILE  | CA   | 66.129     | 0.3         | 1         |
| B     | 31  | ARG  | N    | 119.557    | 0.3         | 1         |
| B     | 5   | ARG  | HA   | 4.594      | 0.05        | 1         |
| B     | 32  | VAL  | HG11 | 0.867      | 0.05        | 2         |
| B     | 38  | MET  | HA   | 4.235      | 0.05        | 1         |
| B     | 38  | MET  | CA   | 59.967     | 0.3         | 1         |
| B     | 53  | GLU  | N    | 125.725    | 0.3         | 1         |
| B     | 25  | ILE  | HG22 | 0.98       | 0.05        | 1         |
| B     | 27  | ALA  | HB1  | 1.656      | 0.05        | 1         |
| B     | 2   | VAL  | HG21 | 1.037      | 0.05        | 2         |
| B     | 18  | VAL  | HG22 | 0.985      | 0.05        | 2         |
| B     | 8   | GLY  | H    | 8.382      | 0.05        | 1         |
| B     | 25  | ILE  | C    | 178.317    | 0.3         | 1         |
| B     | 2   | VAL  | CB   | 32.822     | 0.3         | 1         |
| B     | 47  | LEU  | HG   | 2.009      | 0.05        | 1         |
| B     | 24  | GLU  | CG   | 36.88      | 0.3         | 1         |
| B     | 14  | LYS  | CG   | 24.732     | 0.3         | 1         |
| B     | 21  | TYR  | HE2  | 6.82       | 0.05        | 3         |
| B     | 24  | GLU  | HG3  | 2.42       | 0.05        | 2         |
| B     | 42  | ILE  | HG21 | 0.875      | 0.05        | 1         |
| B     | 18  | VAL  | HG13 | 0.926      | 0.05        | 2         |
| B     | 18  | VAL  | N    | 127.579    | 0.3         | 1         |
| B     | 51  | GLU  | HB3  | 2.139      | 0.05        | 2         |
| B     | 21  | TYR  | CA   | 58.93      | 0.3         | 1         |
| B     | 25  | ILE  | H    | 7.85       | 0.05        | 1         |
| B     | 41  | TYR  | CE2  | 119.0      | 0.3         | 3         |
| B     | 17  | VAL  | N    | 125.65     | 0.3         | 1         |
| B     | 13  | THR  | CA   | 60.358     | 0.3         | 1         |
| B     | 19  | ARG  | HD2  | 3.147      | 0.05        | 2         |
| B     | 42  | ILE  | C    | 178.148    | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 38  | MET  | HB3  | 2.589      | 0.05        | 2         |
| B     | 50  | LEU  | HB2  | 1.617      | 0.05        | 2         |
| B     | 47  | LEU  | CB   | 40.633     | 0.3         | 1         |
| B     | 38  | MET  | N    | 122.4      | 0.3         | 1         |
| B     | 53  | GLU  | CA   | 58.02      | 0.3         | 1         |
| B     | 32  | VAL  | H    | 7.034      | 0.05        | 1         |
| B     | 2   | VAL  | HA   | 4.189      | 0.05        | 1         |
| B     | 28  | LEU  | CD1  | 25.302     | 0.3         | 1         |
| B     | 44  | ARG  | HG3  | 1.762      | 0.05        | 2         |
| B     | 22  | PRO  | HG2  | 2.527      | 0.05        | 2         |
| B     | 3   | GLY  | H    | 8.55       | 0.05        | 1         |
| B     | 26  | GLU  | HG3  | 2.457      | 0.05        | 2         |
| B     | 49  | HIS  | CB   | 29.31      | 0.3         | 1         |
| B     | 20  | LEU  | CD2  | 26.138     | 0.3         | 2         |
| B     | 6   | PRO  | C    | 178.098    | 0.3         | 1         |
| B     | 42  | ILE  | CG2  | 18.327     | 0.3         | 1         |
| B     | 25  | ILE  | HG13 | 0.859      | 0.05        | 2         |
| B     | 27  | ALA  | CB   | 18.527     | 0.3         | 1         |
| B     | 41  | TYR  | CD1  | 132.7      | 0.3         | 3         |
| B     | 43  | ARG  | HB3  | 2.11       | 0.05        | 2         |
| B     | 48  | ASN  | HB3  | 2.95       | 0.05        | 2         |
| B     | 15  | PRO  | HG2  | 2.325      | 0.05        | 2         |
| B     | 52  | ASP  | HB2  | 2.77       | 0.05        | 2         |
| B     | 31  | ARG  | CB   | 31.352     | 0.3         | 1         |
| B     | 14  | LYS  | HG3  | 1.465      | 0.05        | 2         |
| B     | 41  | TYR  | HA   | 4.29       | 0.05        | 1         |
| B     | 16  | VAL  | HG12 | 0.902      | 0.05        | 2         |
| B     | 1   | MET  | CA   | 55.75      | 0.3         | 1         |
| B     | 6   | PRO  | CA   | 63.632     | 0.3         | 1         |
| B     | 23  | ASP  | C    | 179.364    | 0.3         | 1         |
| B     | 37  | SER  | N    | 119.067    | 0.3         | 1         |
| B     | 44  | ARG  | C    | 178.607    | 0.3         | 1         |
| B     | 35  | ASN  | HB3  | 3.12       | 0.05        | 2         |
| B     | 36  | THR  | HB   | 4.121      | 0.05        | 1         |
| B     | 22  | PRO  | HD3  | 3.945      | 0.05        | 2         |
| B     | 16  | VAL  | CG2  | 21.156     | 0.3         | 2         |
| B     | 27  | ALA  | H    | 7.77       | 0.05        | 1         |
| B     | 35  | ASN  | C    | 174.797    | 0.3         | 1         |
| B     | 21  | TYR  | CD2  | 133.4      | 0.3         | 3         |
| B     | 45  | ILE  | HG12 | 1.156      | 0.05        | 2         |
| B     | 44  | ARG  | H    | 7.668      | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 41  | TYR  | H    | 8.48       | 0.05        | 1         |
| B     | 26  | GLU  | HB2  | 2.165      | 0.05        | 2         |
| B     | 49  | HIS  | HB2  | 3.218      | 0.05        | 2         |
| B     | 48  | ASN  | HA   | 4.524      | 0.05        | 1         |
| B     | 37  | SER  | HB2  | 4.476      | 0.05        | 2         |
| B     | 31  | ARG  | H    | 7.763      | 0.05        | 1         |
| B     | 44  | ARG  | CG   | 26.53      | 0.3         | 1         |
| B     | 50  | LEU  | CD2  | 25.659     | 0.3         | 2         |
| B     | 47  | LEU  | HD13 | 0.937      | 0.05        | 2         |
| B     | 17  | VAL  | CB   | 32.841     | 0.3         | 1         |
| B     | 47  | LEU  | CD2  | 21.56      | 0.3         | 2         |
| B     | 39  | SER  | HA   | 4.18       | 0.05        | 1         |
| B     | 35  | ASN  | HD22 | 7.685      | 0.05        | 2         |
| B     | 32  | VAL  | HG22 | 0.812      | 0.05        | 2         |
| B     | 34  | ALA  | C    | 179.218    | 0.3         | 1         |
| B     | 4   | ARG  | HB3  | 1.838      | 0.05        | 2         |
| B     | 16  | VAL  | N    | 124.67     | 0.3         | 1         |
| B     | 32  | VAL  | HG12 | 0.867      | 0.05        | 2         |
| B     | 31  | ARG  | HG2  | 1.829      | 0.05        | 2         |
| B     | 4   | ARG  | HA   | 4.44       | 0.05        | 1         |
| B     | 22  | PRO  | CD   | 51.15      | 0.3         | 1         |
| B     | 19  | ARG  | HB2  | 1.912      | 0.05        | 2         |
| B     | 37  | SER  | CA   | 56.974     | 0.3         | 1         |
| B     | 15  | PRO  | HB2  | 1.867      | 0.05        | 2         |
| B     | 42  | ILE  | HD12 | 0.803      | 0.05        | 1         |
| B     | 43  | ARG  | HG3  | 1.716      | 0.05        | 2         |
| B     | 45  | ILE  | CG2  | 17.699     | 0.3         | 1         |
| B     | 33  | PRO  | HD3  | 3.346      | 0.05        | 2         |
| B     | 29  | LYS  | HG3  | 1.754      | 0.05        | 2         |
| B     | 14  | LYS  | CD   | 29.114     | 0.3         | 1         |
| B     | 5   | ARG  | HB3  | 2.081      | 0.05        | 2         |
| B     | 4   | ARG  | HD2  | 3.224      | 0.05        | 2         |
| B     | 51  | GLU  | CG   | 36.32      | 0.3         | 1         |
| B     | 40  | ALA  | CB   | 18.761     | 0.3         | 1         |
| B     | 34  | ALA  | CA   | 53.93      | 0.3         | 1         |
| B     | 33  | PRO  | CB   | 32.622     | 0.3         | 1         |
| B     | 1   | MET  | HE1  | 2.166      | 0.05        | 1         |
| B     | 26  | GLU  | N    | 118.181    | 0.3         | 1         |
| B     | 3   | GLY  | CA   | 45.39      | 0.3         | 1         |
| B     | 12  | ASP  | H    | 8.187      | 0.05        | 1         |
| B     | 11  | LYS  | H    | 8.354      | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 6   | PRO  | HD3  | 4.204      | 0.05        | 2         |
| B     | 52  | ASP  | CA   | 54.871     | 0.3         | 1         |
| B     | 29  | LYS  | CB   | 32.712     | 0.3         | 1         |
| B     | 16  | VAL  | CA   | 61.845     | 0.3         | 1         |
| B     | 42  | ILE  | CB   | 37.624     | 0.3         | 1         |
| B     | 31  | ARG  | HD2  | 3.209      | 0.05        | 2         |
| B     | 2   | VAL  | HB   | 2.16       | 0.05        | 1         |
| B     | 17  | VAL  | HG22 | 0.99       | 0.05        | 2         |
| B     | 19  | ARG  | C    | 175.687    | 0.3         | 1         |
| B     | 50  | LEU  | H    | 8.196      | 0.05        | 1         |
| B     | 48  | ASN  | HD22 | 7.787      | 0.05        | 2         |
| B     | 17  | VAL  | CG2  | 21.976     | 0.3         | 2         |
| B     | 10  | LEU  | HD22 | 0.907      | 0.05        | 2         |
| B     | 24  | GLU  | HB3  | 1.84       | 0.05        | 2         |
| B     | 1   | MET  | HB2  | 2.06       | 0.05        | 2         |
| B     | 34  | ALA  | N    | 121.917    | 0.3         | 1         |
| B     | 3   | GLY  | HA2  | 4.051      | 0.05        | 2         |
| B     | 45  | ILE  | HD11 | 0.388      | 0.05        | 1         |
| B     | 11  | LYS  | HB3  | 1.99       | 0.05        | 2         |
| B     | 28  | LEU  | N    | 120.403    | 0.3         | 1         |
| B     | 7   | GLY  | N    | 109.847    | 0.3         | 1         |
| B     | 43  | ARG  | CD   | 43.059     | 0.3         | 1         |
| B     | 45  | ILE  | HG23 | 0.576      | 0.05        | 1         |
| B     | 29  | LYS  | HE2  | 2.985      | 0.05        | 2         |
| B     | 36  | THR  | HG23 | 1.469      | 0.05        | 1         |
| B     | 1   | MET  | HG2  | 2.53       | 0.05        | 2         |
| B     | 15  | PRO  | CD   | 50.446     | 0.3         | 1         |
| B     | 25  | ILE  | CG1  | 30.95      | 0.3         | 1         |
| B     | 29  | LYS  | HA   | 3.858      | 0.05        | 1         |
| B     | 47  | LEU  | HD21 | 0.948      | 0.05        | 2         |
| B     | 6   | PRO  | CD   | 50.879     | 0.3         | 1         |
| B     | 42  | ILE  | HA   | 3.501      | 0.05        | 1         |
| B     | 28  | LEU  | HD23 | 1.093      | 0.05        | 2         |
| B     | 11  | LYS  | HG2  | 1.55       | 0.05        | 2         |
| B     | 10  | LEU  | CA   | 56.244     | 0.3         | 1         |
| B     | 16  | VAL  | CG1  | 21.088     | 0.3         | 2         |
| B     | 30  | SER  | CA   | 60.922     | 0.3         | 1         |
| B     | 28  | LEU  | HD11 | 1.031      | 0.05        | 2         |
| B     | 46  | ILE  | HG21 | 0.993      | 0.05        | 1         |
| B     | 28  | LEU  | CA   | 58.251     | 0.3         | 1         |
| B     | 46  | ILE  | HD13 | 0.925      | 0.05        | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 50  | LEU  | CD1  | 22.47      | 0.3         | 2         |
| B     | 20  | LEU  | HD13 | 1.01       | 0.05        | 2         |
| B     | 39  | SER  | HB3  | 4.076      | 0.05        | 2         |
| B     | 35  | ASN  | H    | 8.684      | 0.05        | 1         |
| B     | 22  | PRO  | CA   | 67.002     | 0.3         | 1         |
| B     | 4   | ARG  | HG3  | 1.665      | 0.05        | 2         |
| B     | 1   | MET  | CE   | 17.265     | 0.3         | 1         |
| B     | 11  | LYS  | CG   | 24.87      | 0.3         | 1         |
| B     | 42  | ILE  | HD11 | 0.803      | 0.05        | 1         |
| B     | 38  | MET  | H    | 9.125      | 0.05        | 1         |
| B     | 8   | GLY  | HA3  | 4.13       | 0.05        | 2         |
| B     | 33  | PRO  | HG3  | 2.228      | 0.05        | 2         |
| B     | 11  | LYS  | HD3  | 1.778      | 0.05        | 2         |
| B     | 25  | ILE  | CA   | 66.024     | 0.3         | 1         |
| B     | 51  | GLU  | CB   | 30.26      | 0.3         | 1         |
| B     | 51  | GLU  | HA   | 4.312      | 0.05        | 1         |
| B     | 35  | ASN  | HA   | 4.594      | 0.05        | 1         |
| B     | 34  | ALA  | CB   | 18.533     | 0.3         | 1         |
| B     | 33  | PRO  | CG   | 27.506     | 0.3         | 1         |
| B     | 50  | LEU  | HD13 | 0.89       | 0.05        | 2         |
| B     | 53  | GLU  | HA   | 4.22       | 0.05        | 1         |
| B     | 34  | ALA  | HB3  | 1.49       | 0.05        | 1         |
| B     | 18  | VAL  | CB   | 34.369     | 0.3         | 1         |
| B     | 22  | PRO  | HB3  | 2.05       | 0.05        | 2         |
| B     | 35  | ASN  | CB   | 37.83      | 0.3         | 1         |
| B     | 19  | ARG  | CG   | 26.91      | 0.3         | 1         |
| B     | 34  | ALA  | HA   | 4.227      | 0.05        | 1         |
| B     | 29  | LYS  | C    | 179.54     | 0.3         | 1         |
| B     | 52  | ASP  | CB   | 41.57      | 0.3         | 1         |
| B     | 29  | LYS  | CG   | 26.135     | 0.3         | 1         |
| B     | 42  | ILE  | CA   | 66.02      | 0.3         | 1         |
| B     | 47  | LEU  | N    | 120.336    | 0.3         | 1         |
| B     | 20  | LEU  | C    | 176.68     | 0.3         | 1         |
| B     | 38  | MET  | CB   | 32.376     | 0.3         | 1         |
| B     | 25  | ILE  | HG23 | 0.98       | 0.05        | 1         |
| B     | 4   | ARG  | C    | 176.599    | 0.3         | 1         |
| B     | 27  | ALA  | HB2  | 1.656      | 0.05        | 1         |
| B     | 25  | ILE  | CD1  | 13.64      | 0.3         | 1         |
| B     | 10  | LEU  | HB2  | 1.762      | 0.05        | 2         |
| B     | 18  | VAL  | HG21 | 0.985      | 0.05        | 2         |
| B     | 2   | VAL  | CA   | 62.709     | 0.3         | 1         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 46  | ILE  | HG12 | 1.943      | 0.05        | 2         |
| B     | 41  | TYR  | HE1  | 6.798      | 0.05        | 3         |
| B     | 25  | ILE  | N    | 119.2      | 0.3         | 1         |
| B     | 25  | ILE  | HD12 | 0.85       | 0.05        | 1         |
| B     | 10  | LEU  | H    | 8.328      | 0.05        | 1         |
| B     | 45  | ILE  | HD12 | 0.388      | 0.05        | 1         |
| B     | 51  | GLU  | HB2  | 2.204      | 0.05        | 2         |
| B     | 27  | ALA  | N    | 121.839    | 0.3         | 1         |
| B     | 41  | TYR  | CE1  | 119.0      | 0.3         | 3         |
| B     | 28  | LEU  | HB3  | 1.817      | 0.05        | 2         |
| B     | 50  | LEU  | HB3  | 2.069      | 0.05        | 2         |
| B     | 2   | VAL  | C    | 177.021    | 0.3         | 1         |
| B     | 15  | PRO  | CA   | 62.351     | 0.3         | 1         |
| B     | 41  | TYR  | HB3  | 3.25       | 0.05        | 2         |
| B     | 2   | VAL  | HG11 | 1.037      | 0.05        | 2         |
| B     | 25  | ILE  | CG2  | 17.32      | 0.3         | 1         |
| B     | 44  | ARG  | HB3  | 1.98       | 0.05        | 2         |
| B     | 6   | PRO  | CG   | 27.751     | 0.3         | 1         |
| B     | 28  | LEU  | CD2  | 24.676     | 0.3         | 1         |
| B     | 13  | THR  | HG23 | 0.317      | 0.05        | 1         |
| B     | 23  | ASP  | CA   | 56.871     | 0.3         | 1         |
| B     | 10  | LEU  | CB   | 42.353     | 0.3         | 1         |
| B     | 53  | GLU  | HB3  | 2.118      | 0.05        | 2         |
| B     | 42  | ILE  | CG1  | 29.985     | 0.3         | 1         |
| B     | 25  | ILE  | HG12 | 1.796      | 0.05        | 2         |
| B     | 25  | ILE  | HB   | 2.071      | 0.05        | 1         |
| B     | 28  | LEU  | HA   | 4.126      | 0.05        | 1         |
| B     | 41  | TYR  | CD2  | 132.7      | 0.3         | 3         |
| B     | 14  | LYS  | H    | 9.064      | 0.05        | 1         |
| B     | 35  | ASN  | N    | 114.379    | 0.3         | 1         |
| B     | 35  | ASN  | HD21 | 6.966      | 0.05        | 2         |
| B     | 38  | MET  | HE3  | 2.233      | 0.05        | 1         |
| B     | 48  | ASN  | HB2  | 2.912      | 0.05        | 2         |
| B     | 52  | ASP  | HB3  | 2.88       | 0.05        | 2         |
| B     | 31  | ARG  | CA   | 55.41      | 0.3         | 1         |
| B     | 14  | LYS  | HG2  | 1.563      | 0.05        | 2         |
| B     | 13  | THR  | H    | 7.615      | 0.05        | 1         |
| B     | 27  | ALA  | HA   | 4.26       | 0.05        | 1         |
| B     | 49  | HIS  | CA   | 59.101     | 0.3         | 1         |
| B     | 22  | PRO  | CB   | 32.334     | 0.3         | 1         |
| B     | 16  | VAL  | HG13 | 0.902      | 0.05        | 2         |

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| Chain | Res | Type | Atom | Shift Data |             |           |
|-------|-----|------|------|------------|-------------|-----------|
|       |     |      |      | Value      | Uncertainty | Ambiguity |
| B     | 17  | VAL  | HG13 | 0.83       | 0.05        | 2         |
| B     | 35  | ASN  | HB2  | 3.005      | 0.05        | 2         |
| B     | 36  | THR  | HA   | 4.635      | 0.05        | 1         |
| B     | 7   | GLY  | HA2  | 4.09       | 0.05        | 2         |
| B     | 21  | TYR  | HA   | 4.65       | 0.05        | 1         |

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 156      | $-0.51 \pm 0.19$                | Should be applied          |
| $^{13}\text{C}_\beta$  | 147      | $0.14 \pm 0.13$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}'$       | 105      | $-0.64 \pm 0.15$                | Should be applied          |
| $^{15}\text{N}$        | 144      | $0.04 \pm 0.26$                 | None needed ( $< 0.5$ ppm) |

### 7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 85%, i.e. 928 atoms were assigned a chemical shift out of a possible 1092. 2 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total          | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|----------------|---------------|-----------------|-----------------|
| Backbone  | 378/408 (93%)  | 158/162 (98%) | 142/168 (85%)   | 78/78 (100%)    |
| Sidechain | 514/636 (81%)  | 316/372 (85%) | 194/231 (84%)   | 4/33 (12%)      |
| Aromatic  | 36/48 (75%)    | 18/24 (75%)   | 18/20 (90%)     | 0/4 (0%)        |
| Overall   | 928/1092 (85%) | 492/558 (88%) | 354/419 (84%)   | 82/115 (71%)    |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1132 atoms were assigned a chemical shift out of a possible 1354. 2 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total           | $^1\text{H}$  | $^{13}\text{C}$ | $^{15}\text{N}$ |
|-----------|-----------------|---------------|-----------------|-----------------|
| Backbone  | 468/514 (91%)   | 198/204 (97%) | 174/212 (82%)   | 96/98 (98%)     |
| Sidechain | 628/792 (79%)   | 386/466 (83%) | 238/280 (85%)   | 4/46 (9%)       |
| Aromatic  | 36/48 (75%)     | 18/24 (75%)   | 18/20 (90%)     | 0/4 (0%)        |
| Overall   | 1132/1354 (84%) | 602/694 (87%) | 430/512 (84%)   | 100/148 (68%)   |

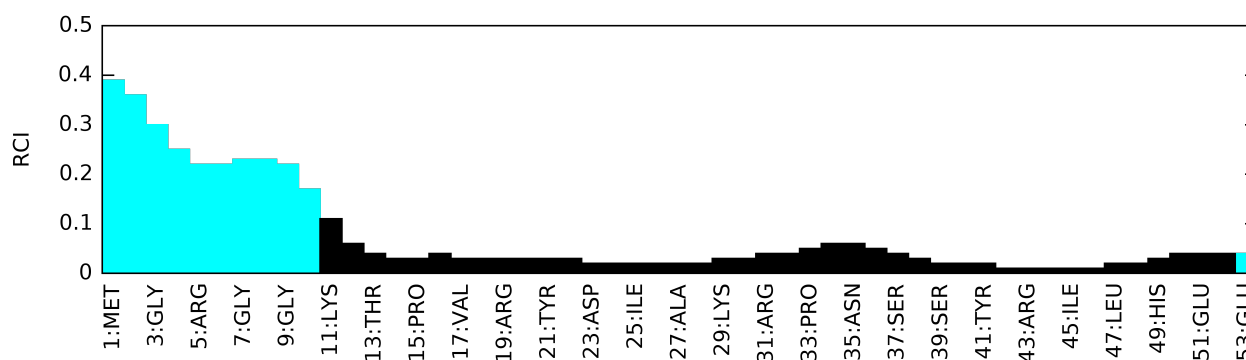
### 7.1.4 Statistically unusual chemical shifts [i](#)

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:

