



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 4, 2025 – 02:23 PM EST

PDB ID : 8EPY  
BMRB ID : 31046  
Title : The solution structure of abxF in complex with its product (-)-ABX, an enzyme catalyzing the formation of the chiral spiroketal of an anthrabenzoxocinone antibiotic, (-)-ABX  
Authors : Jia, X.; Yan, X.; Qu, X.; Mobli, M.  
Deposited on : 2022-10-06

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

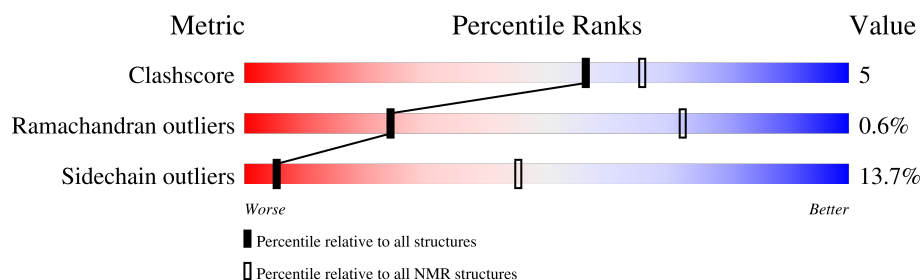
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 4%.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 210492                      | 14027                     |
| Ramachandran outliers | 207382                      | 12486                     |
| Sidechain outliers    | 206894                      | 12463                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 245    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:16-A:41, A:51-A:132,<br>A:141-A:166, A:183-A:245<br>(197) | 0.42              | 2            |

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

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

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

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

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

There are 2 unique types of molecules in this entry. The entry contains 3521 atoms, of which 1714 are hydrogens and 0 are deuteriums.

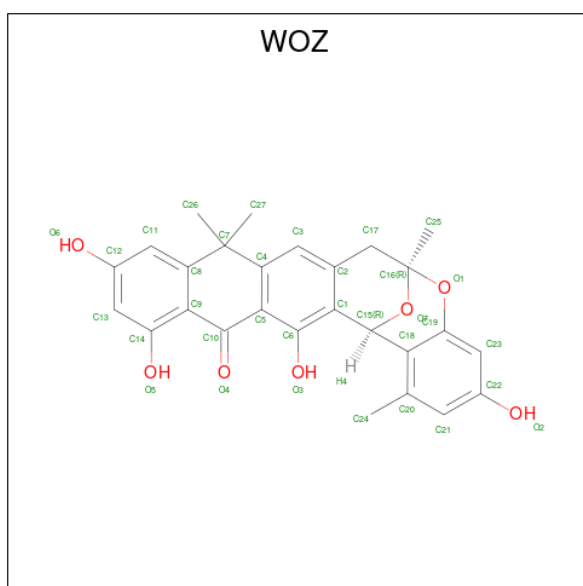
- Molecule 1 is a protein called Glyoxalase.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|-------|
|     |       |          | Total | C    | H    | N   | O   | S |       |
| 1   | A     | 245      | 3463  | 1110 | 1690 | 307 | 348 | 8 | 0     |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| A     | 1       | GLY      | -      | expression tag | UNP A0A2I6B3F9 |
| A     | 2       | SER      | -      | expression tag | UNP A0A2I6B3F9 |
| A     | 3       | HIS      | -      | expression tag | UNP A0A2I6B3F9 |

- Molecule 2 is (6R,16R)-3,11,13,15-tetrahydroxy-1,6,9,9-tetramethyl-6,7,9,16-tetrahydro-14H-6,16-epoxyanthra[2,3-e]benzo[b]oxocin-14-one (three-letter code: WOZ) (formula:  $C_{27}H_{24}O_7$ ) (labeled as "Ligand of Interest" by depositor).



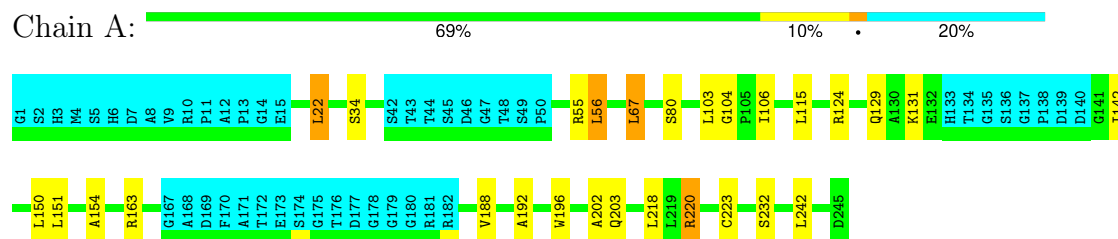
| Mol | Chain | Residues | Atoms |    |    |   |
|-----|-------|----------|-------|----|----|---|
|     |       |          | Total | C  | H  | O |
| 2   | A     | 1        | 58    | 27 | 24 | 7 |

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

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

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

- Molecule 1: Glyoxalase

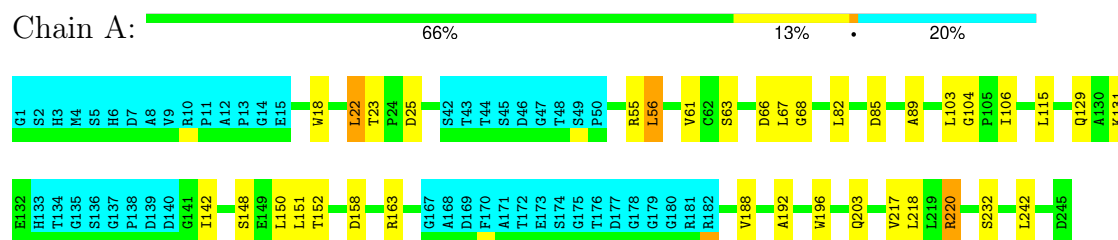


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

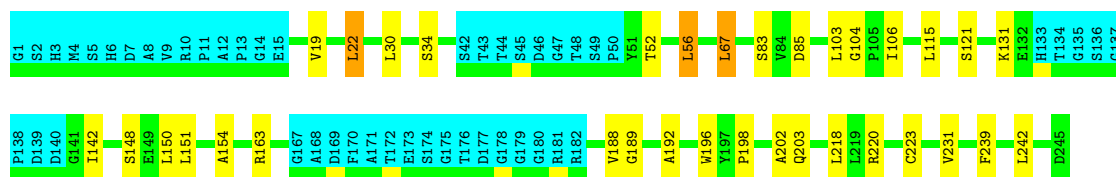
- Molecule 1: Glyoxalase



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

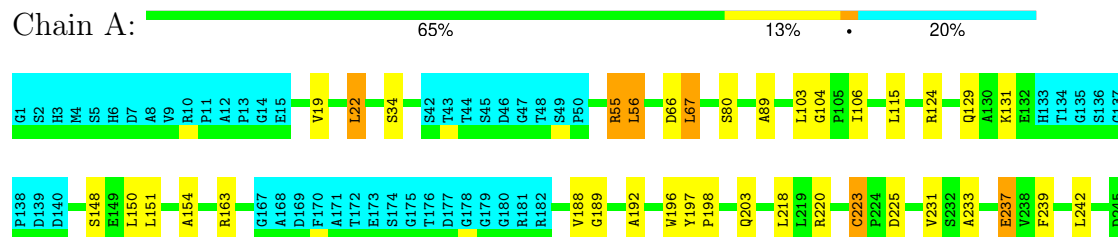
- Molecule 1: Glyoxalase





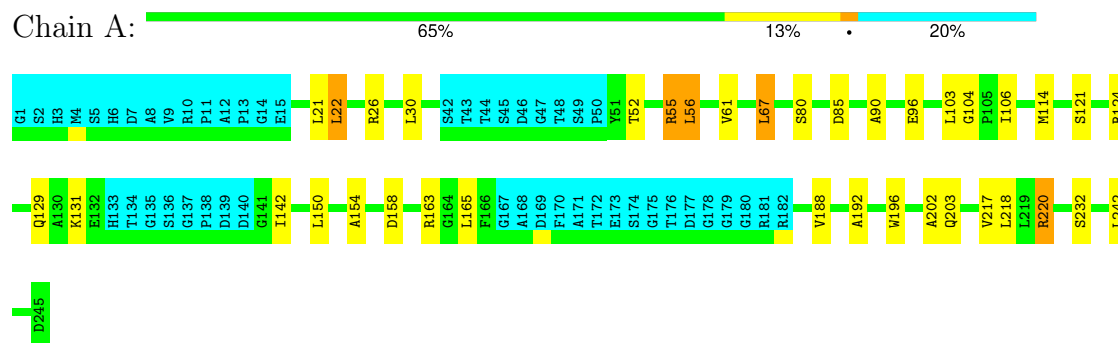
### 4.2.3 Score per residue for model 3

- Molecule 1: Glyoxalase



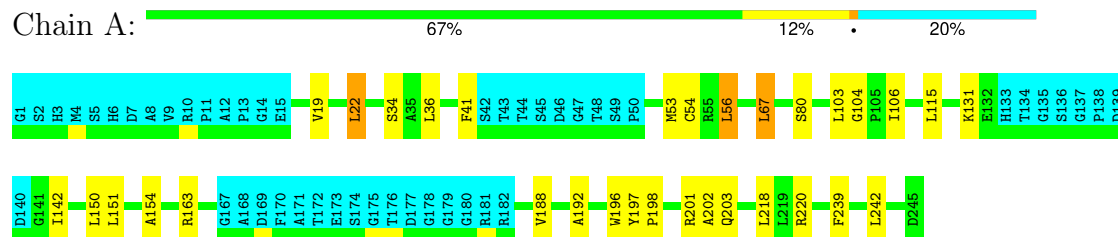
### 4.2.4 Score per residue for model 4

- Molecule 1: Glyoxalase

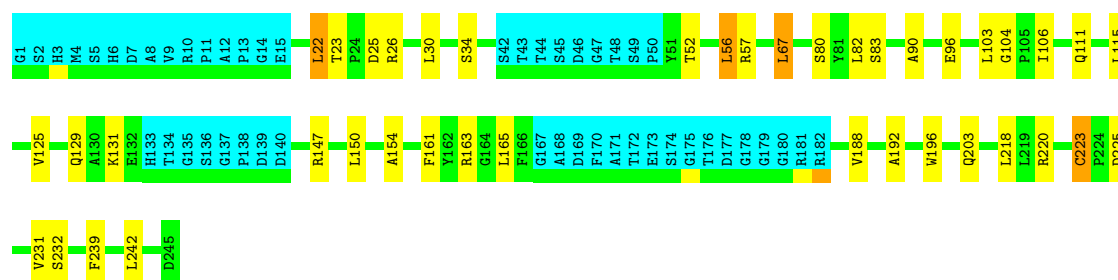


### 4.2.5 Score per residue for model 5

- Molecule 1: Glyoxalase

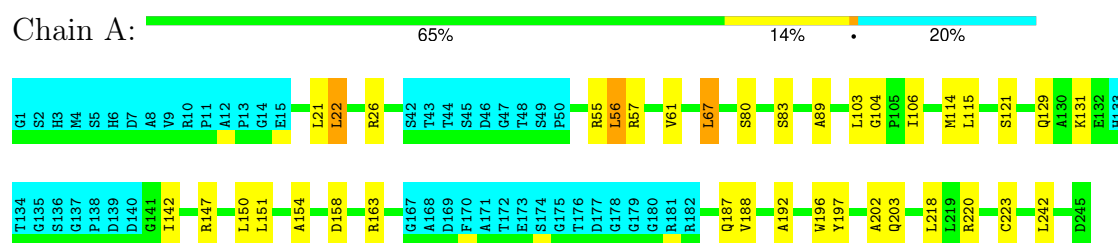






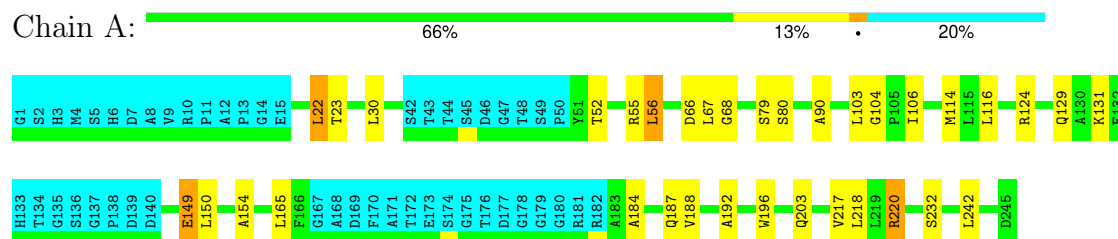
#### 4.2.10 Score per residue for model 10

- Molecule 1: Glyoxalase



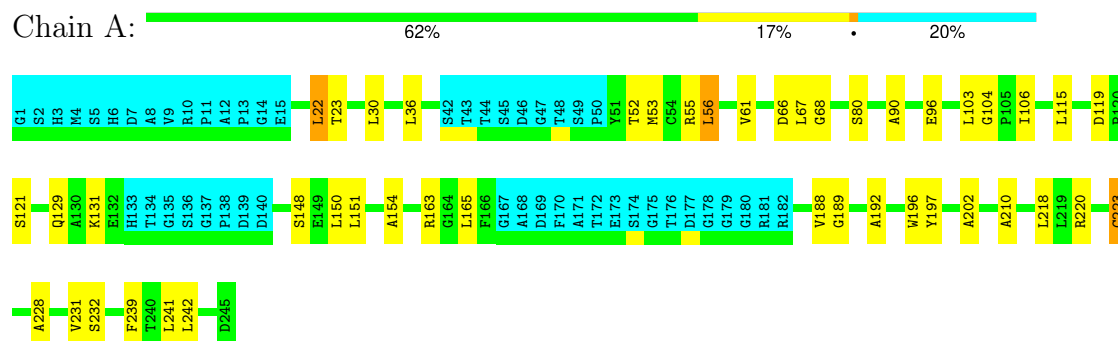
#### 4.2.11 Score per residue for model 11

- Molecule 1: Glyoxalase



#### 4.2.12 Score per residue for model 12

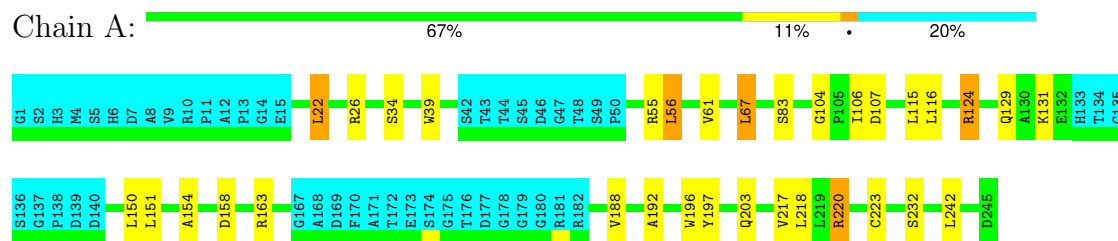
- Molecule 1: Glyoxalase





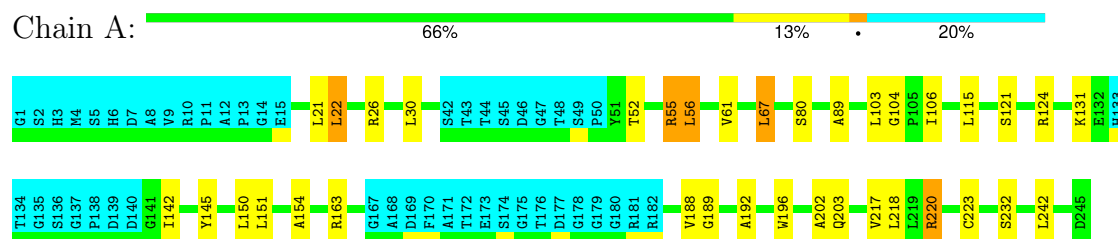
### 4.2.13 Score per residue for model 13

- Molecule 1: Glyoxalase



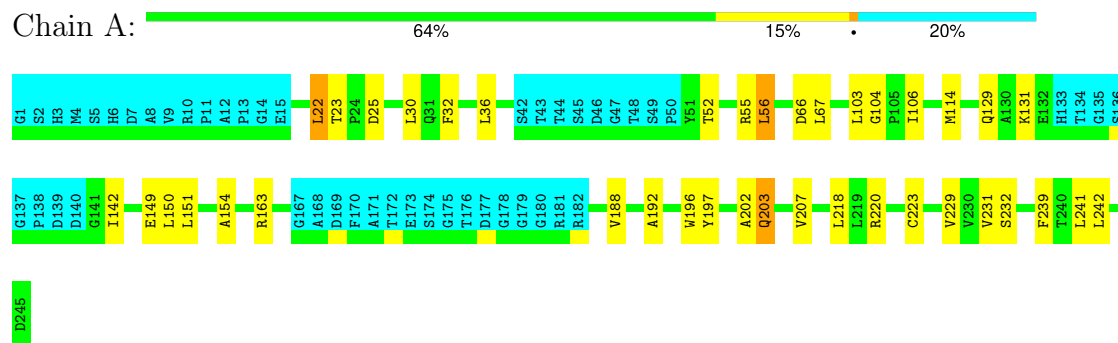
### 4.2.14 Score per residue for model 14

- Molecule 1: Glyoxalase



### 4.2.15 Score per residue for model 15

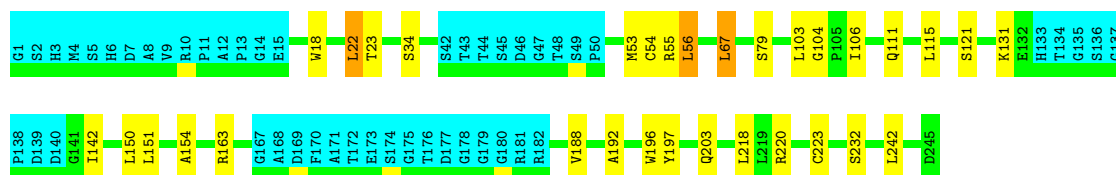
- Molecule 1: Glyoxalase



### 4.2.16 Score per residue for model 16

- Molecule 1: Glyoxalase

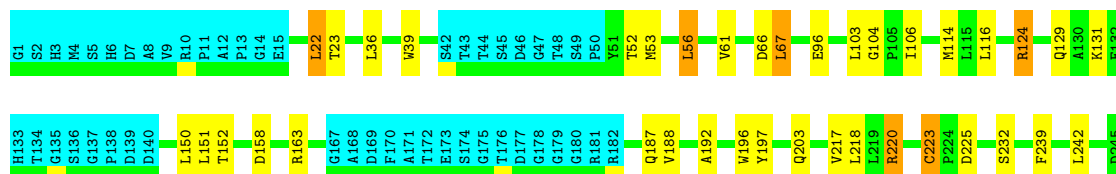




#### 4.2.17 Score per residue for model 17

- Molecule 1: Glyoxalase

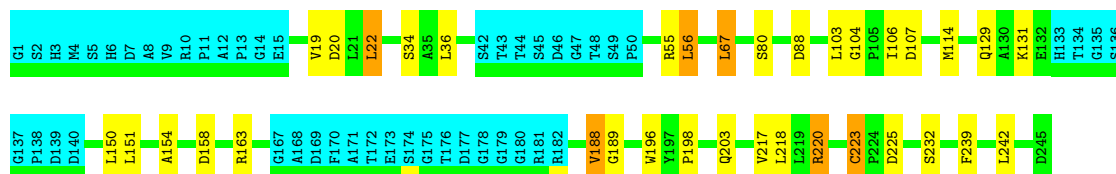
Chain A: 65% 13% 20%



#### 4.2.18 Score per residue for model 18

- Molecule 1: Glyoxalase

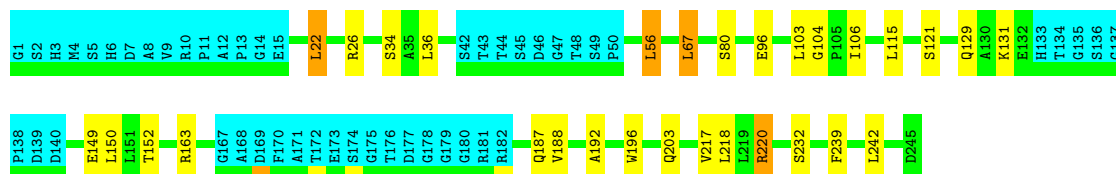
Chain A: 66% 12% 20%



#### 4.2.19 Score per residue for model 19

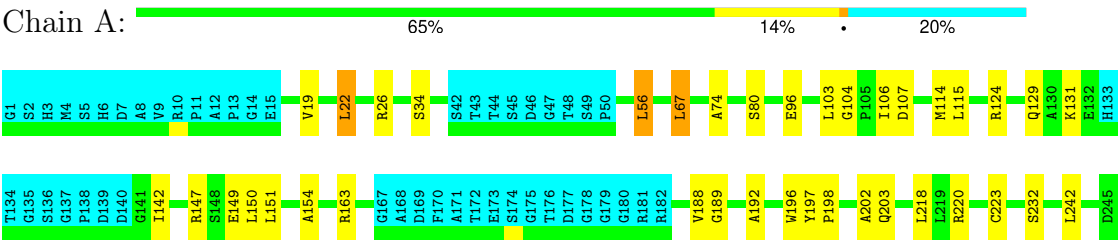
- Molecule 1: Glyoxalase

Chain A: 68% 11% 20%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Glyoxalase



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

| Software name | Classification        | Version |
|---------------|-----------------------|---------|
| CYANA         | structure calculation |         |
| XTB           | refinement            |         |

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

|  |                |
|--|----------------|
| Chemical shift file(s)                       | working_cs.cif |
| Number of chemical shift lists               | 1              |
| Total number of shifts                       | 2684           |
| Number of shifts mapped to atoms             | 140            |
| Number of unparsed shifts                    | 0              |
| Number of shifts with mapping errors         | 2544           |
| Number of shifts with mapping warnings       | 0              |
| Assignment completeness (well-defined parts) | 4%             |

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

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 [i](#)

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     | 1446  | 1410     | 1410     | 14±2    |
| All | All   | 29600 | 28680    | 28200    | 274     |

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 5.

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

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:22:LEU:HD23  | 1:A:67:LEU:HD12  | 0.72     | 1.62        | 13     | 15    |
| 1:A:22:LEU:HD23  | 1:A:67:LEU:HD22  | 0.62     | 1.72        | 15     | 1     |
| 1:A:22:LEU:HD22  | 1:A:22:LEU:C     | 0.58     | 2.19        | 15     | 20    |
| 1:A:67:LEU:HD13  | 1:A:67:LEU:N     | 0.57     | 2.14        | 16     | 15    |
| 1:A:188:VAL:HB   | 1:A:192:ALA:HB3  | 0.56     | 1.78        | 11     | 19    |
| 1:A:30:LEU:HD21  | 1:A:52:THR:HG21  | 0.55     | 1.77        | 15     | 7     |
| 1:A:90:ALA:HB1   | 1:A:165:LEU:HD23 | 0.55     | 1.78        | 9      | 1     |
| 1:A:36:LEU:HD13  | 1:A:239:PHE:CZ   | 0.54     | 2.37        | 19     | 4     |
| 1:A:202:ALA:HB3  | 1:A:241:LEU:HD23 | 0.54     | 1.78        | 15     | 1     |
| 1:A:142:ILE:HG21 | 1:A:203:GLN:OE1  | 0.53     | 2.03        | 20     | 3     |
| 1:A:150:LEU:HD13 | 1:A:196:TRP:CD1  | 0.53     | 2.38        | 15     | 20    |
| 1:A:116:LEU:HD13 | 1:A:124:ARG:HG3  | 0.53     | 1.81        | 17     | 2     |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Clash(Å) | Distance(Å) | Models |       |
|------------------|------------------|----------|-------------|--------|-------|
|                  |                  |          |             | Worst  | Total |
| 1:A:104:GLY:HA2  | 1:A:106:ILE:HG23 | 0.52     | 1.80        | 3      | 20    |
| 1:A:217:VAL:HG13 | 1:A:220:ARG:NE   | 0.52     | 2.20        | 4      | 10    |
| 1:A:56:LEU:HD13  | 1:A:56:LEU:N     | 0.51     | 2.20        | 8      | 20    |
| 1:A:116:LEU:HD13 | 1:A:124:ARG:HD2  | 0.51     | 1.83        | 11     | 1     |
| 1:A:19:VAL:HG11  | 1:A:198:PRO:HG3  | 0.50     | 1.82        | 8      | 6     |
| 1:A:233:ALA:HB3  | 1:A:237:GLU:HG3  | 0.50     | 1.83        | 3      | 1     |
| 1:A:55:ARG:C     | 1:A:56:LEU:HD13  | 0.48     | 2.29        | 12     | 13    |
| 1:A:142:ILE:HG23 | 1:A:202:ALA:HA   | 0.47     | 1.85        | 20     | 9     |
| 1:A:22:LEU:O     | 1:A:22:LEU:HD13  | 0.47     | 2.09        | 4      | 15    |
| 1:A:67:LEU:HD12  | 1:A:68:GLY:N     | 0.47     | 2.25        | 1      | 4     |
| 1:A:151:LEU:HD23 | 1:A:197:TYR:CE2  | 0.47     | 2.45        | 8      | 10    |
| 1:A:77:GLY:HA2   | 1:A:237:GLU:OE1  | 0.47     | 2.10        | 6      | 1     |
| 1:A:56:LEU:HD11  | 1:A:61:VAL:HG21  | 0.46     | 1.85        | 4      | 3     |
| 1:A:90:ALA:HB1   | 1:A:165:LEU:HD13 | 0.46     | 1.86        | 12     | 3     |
| 1:A:22:LEU:HD22  | 1:A:23:THR:N     | 0.46     | 2.25        | 8      | 9     |
| 1:A:231:VAL:HG23 | 1:A:239:PHE:CZ   | 0.46     | 2.46        | 12     | 5     |
| 1:A:39:TRP:CZ2   | 1:A:61:VAL:HG11  | 0.46     | 2.46        | 13     | 3     |
| 1:A:56:LEU:HD11  | 1:A:61:VAL:HG11  | 0.45     | 1.86        | 7      | 2     |
| 1:A:149:GLU:HB3  | 1:A:184:ALA:HB3  | 0.45     | 1.86        | 11     | 1     |
| 1:A:125:VAL:HG11 | 1:A:161:PHE:CE2  | 0.45     | 2.47        | 9      | 1     |
| 1:A:151:LEU:HD12 | 1:A:188:VAL:CG2  | 0.45     | 2.42        | 18     | 10    |
| 1:A:151:LEU:HD12 | 1:A:188:VAL:HG21 | 0.45     | 1.89        | 1      | 1     |
| 1:A:116:LEU:HD13 | 1:A:124:ARG:CG   | 0.45     | 2.42        | 13     | 1     |
| 1:A:25:ASP:C     | 1:A:25:ASP:OD1   | 0.43     | 2.56        | 9      | 3     |
| 1:A:207:VAL:HG22 | 1:A:229:VAL:HG11 | 0.43     | 1.90        | 15     | 1     |
| 1:A:32:PHE:CE1   | 1:A:36:LEU:HD11  | 0.42     | 2.50        | 15     | 1     |
| 1:A:223:CYS:HB3  | 1:A:225:ASP:OD1  | 0.42     | 2.15        | 18     | 4     |
| 1:A:223:CYS:SG   | 1:A:228:ALA:HB2  | 0.41     | 2.56        | 12     | 1     |
| 1:A:74:ALA:HB1   | 1:A:114:MET:HE1  | 0.41     | 1.92        | 20     | 1     |
| 1:A:202:ALA:HB3  | 1:A:241:LEU:HD12 | 0.41     | 1.91        | 12     | 1     |
| 1:A:41:PHE:CE2   | 1:A:54:CYS:HB2   | 0.41     | 2.51        | 5      | 1     |
| 1:A:36:LEU:HD22  | 1:A:210:ALA:HB2  | 0.41     | 1.93        | 12     | 1     |
| 1:A:22:LEU:HD13  | 1:A:22:LEU:O     | 0.41     | 2.16        | 15     | 1     |
| 1:A:61:VAL:O     | 1:A:145:TYR:CZ   | 0.40     | 2.75        | 14     | 1     |
| 1:A:142:ILE:HD13 | 1:A:203:GLN:HG3  | 0.40     | 1.92        | 15     | 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     | 196/245 (80%)   | 179±2 (91±1%) | 16±2 (8±1%) | 1±1 (1±0%) | 24          | 72 |
| All | All   | 3920/4900 (80%) | 3581 (91%)    | 316 (8%)    | 23 (1%)    | 24          | 72 |

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 154 | ALA  | 17             |
| 1   | A     | 189 | GLY  | 6              |

### 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     | 142/176 (81%)   | 123±2 (86±2%) | 19±2 (14±2%) | 5           | 45 |
| All | All   | 2840/3520 (81%) | 2451 (86%)    | 389 (14%)    | 5           | 45 |

All 47 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 22  | LEU  | 20             |
| 1   | A     | 56  | LEU  | 20             |
| 1   | A     | 131 | LYS  | 20             |
| 1   | A     | 218 | LEU  | 20             |
| 1   | A     | 220 | ARG  | 20             |
| 1   | A     | 242 | LEU  | 20             |
| 1   | A     | 103 | LEU  | 19             |
| 1   | A     | 163 | ARG  | 19             |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 232 | SER  | 16             |
| 1   | A     | 115 | LEU  | 15             |
| 1   | A     | 129 | GLN  | 15             |
| 1   | A     | 67  | LEU  | 15             |
| 1   | A     | 203 | GLN  | 15             |
| 1   | A     | 223 | CYS  | 14             |
| 1   | A     | 80  | SER  | 13             |
| 1   | A     | 34  | SER  | 12             |
| 1   | A     | 26  | ARG  | 9              |
| 1   | A     | 66  | ASP  | 7              |
| 1   | A     | 158 | ASP  | 7              |
| 1   | A     | 121 | SER  | 7              |
| 1   | A     | 124 | ARG  | 7              |
| 1   | A     | 96  | GLU  | 7              |
| 1   | A     | 114 | MET  | 6              |
| 1   | A     | 149 | GLU  | 6              |
| 1   | A     | 148 | SER  | 5              |
| 1   | A     | 53  | MET  | 5              |
| 1   | A     | 85  | ASP  | 4              |
| 1   | A     | 83  | SER  | 4              |
| 1   | A     | 55  | ARG  | 4              |
| 1   | A     | 147 | ARG  | 4              |
| 1   | A     | 187 | GLN  | 4              |
| 1   | A     | 152 | THR  | 3              |
| 1   | A     | 21  | LEU  | 3              |
| 1   | A     | 119 | ASP  | 3              |
| 1   | A     | 79  | SER  | 3              |
| 1   | A     | 107 | ASP  | 3              |
| 1   | A     | 18  | TRP  | 2              |
| 1   | A     | 88  | ASP  | 2              |
| 1   | A     | 57  | ARG  | 2              |
| 1   | A     | 111 | GLN  | 2              |
| 1   | A     | 63  | SER  | 1              |
| 1   | A     | 237 | GLU  | 1              |
| 1   | A     | 201 | ARG  | 1              |
| 1   | A     | 155 | SER  | 1              |
| 1   | A     | 54  | CYS  | 1              |
| 1   | A     | 20  | ASP  | 1              |
| 1   | A     | 188 | VAL  | 1              |



### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths |           |            |
|-----|------|-------|-----|------|--------------|-----------|------------|
|     |      |       |     |      | Counts       | RMSZ      | #Z>2       |
| 2   | WOZ  | A     | 246 | -    | 39,39,39     | 0.69±0.02 | 0±0 (0±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles |           |            |
|-----|------|-------|-----|------|-------------|-----------|------------|
|     |      |       |     |      | Counts      | RMSZ      | #Z>2       |
| 2   | WOZ  | A     | 246 | -    | 54,65,65    | 0.90±0.04 | 3±0 (5±0%) |

All unique bond outliers are listed below.

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(Å) | Ideal(Å) | Models |       |
|-----|-------|-----|------|---------|------|-------------|----------|--------|-------|
|     |       |     |      |         |      |             |          | Worst  | Total |
| 2   | A     | 246 | WOZ  | C25-C16 | 2.16 | 1.53        | 1.51     | 16     | 3     |

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

| Mol | Chain | Res | Type | Atoms       | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-------------|------|-------------|----------|--------|-------|
|     |       |     |      |             |      |             |          | Worst  | Total |
| 2   | A     | 246 | WOZ  | C18-C15-C1  | 3.06 | 114.83      | 110.08   | 4      | 20    |
| 2   | A     | 246 | WOZ  | C16-O1-C19  | 2.67 | 114.13      | 118.47   | 13     | 20    |
| 2   | A     | 246 | WOZ  | C8-C7-C4    | 2.28 | 114.07      | 108.98   | 9      | 19    |
| 2   | A     | 246 | WOZ  | C25-C16-C17 | 2.05 | 111.04      | 113.32   | 17     | 2     |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 4% for the well-defined parts and 5% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 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                  | 2684 |
| Number of shifts mapped to atoms        | 140  |
| Number of unparsed shifts               | 0    |
| Number of shifts with mapping errors    | 2544 |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 5    |

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

- No matching atom found in the structure. All 2544 occurrences are reported below.

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 0   | HIS  | CA   | 56.215     | 0.000       | .         |
| 1       | A     | 0   | HIS  | CB   | 30.083     | 0.000       | .         |
| 1       | A     | 0   | HIS  | CD2  | 119.954    | 0.000       | .         |
| 1       | A     | 0   | HIS  | HD2  | 7.128      | 0.000       | .         |
| 1       | A     | 0   | HIS  | C    | 174.962    | 0.000       | .         |
| 1       | A     | 1   | MET  | N    | 121.713    | 0.000       | .         |
| 1       | A     | 1   | MET  | H    | 8.382      | 0.000       | .         |
| 1       | A     | 1   | MET  | CA   | 55.446     | 0.000       | .         |
| 1       | A     | 1   | MET  | HA   | 4.479      | 0.000       | .         |
| 1       | A     | 1   | MET  | CB   | 32.985     | 0.001       | .         |
| 1       | A     | 1   | MET  | HB2  | 1.941      | 0.000       | .         |
| 1       | A     | 1   | MET  | HB3  | 2.042      | 0.000       | .         |
| 1       | A     | 1   | MET  | CG   | 31.873     | 0.000       | .         |
| 1       | A     | 1   | MET  | HG2  | 2.443      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 1   | MET  | HG3  | 2.512      | 0.000       | .         |
| 1       | A     | 1   | MET  | C    | 176.041    | 0.001       | .         |
| 1       | A     | 4   | ASP  | N    | 120.948    | 0.000       | .         |
| 1       | A     | 4   | ASP  | H    | 8.284      | 0.000       | .         |
| 1       | A     | 4   | ASP  | CA   | 54.433     | 0.000       | .         |
| 1       | A     | 4   | ASP  | HA   | 4.572      | 0.000       | .         |
| 1       | A     | 4   | ASP  | CB   | 41.249     | 0.000       | .         |
| 1       | A     | 4   | ASP  | HB2  | 2.574      | 0.000       | .         |
| 1       | A     | 4   | ASP  | HB3  | 2.672      | 0.000       | .         |
| 1       | A     | 4   | ASP  | C    | 175.69     | 0.000       | .         |
| 1       | A     | 5   | ALA  | N    | 124.02     | 0.000       | .         |
| 1       | A     | 5   | ALA  | H    | 8.143      | 0.000       | .         |
| 1       | A     | 5   | ALA  | CA   | 52.416     | 0.000       | .         |
| 1       | A     | 5   | ALA  | HA   | 4.353      | 0.000       | .         |
| 1       | A     | 5   | ALA  | HB1  | 1.377      | 0.000       | .         |
| 1       | A     | 5   | ALA  | HB2  | 1.377      | 0.000       | .         |
| 1       | A     | 5   | ALA  | HB3  | 1.377      | 0.000       | .         |
| 1       | A     | 5   | ALA  | CB   | 19.401     | 0.000       | .         |
| 1       | A     | 5   | ALA  | C    | 177.369    | 0.002       | .         |
| 1       | A     | 6   | VAL  | N    | 120.034    | 0.000       | .         |
| 1       | A     | 6   | VAL  | H    | 8.157      | 0.000       | .         |
| 1       | A     | 6   | VAL  | CA   | 62.237     | 0.000       | .         |
| 1       | A     | 6   | VAL  | HA   | 4.118      | 0.000       | .         |
| 1       | A     | 6   | VAL  | CB   | 32.741     | 0.000       | .         |
| 1       | A     | 6   | VAL  | HB   | 2.069      | 0.000       | .         |
| 1       | A     | 6   | VAL  | HG11 | 0.937      | 0.005       | .         |
| 1       | A     | 6   | VAL  | HG12 | 0.937      | 0.005       | .         |
| 1       | A     | 6   | VAL  | HG13 | 0.937      | 0.005       | .         |
| 1       | A     | 6   | VAL  | HG21 | 0.935      | 0.000       | .         |
| 1       | A     | 6   | VAL  | HG22 | 0.935      | 0.000       | .         |
| 1       | A     | 6   | VAL  | HG23 | 0.935      | 0.000       | .         |
| 1       | A     | 6   | VAL  | CG1  | 20.654     | 0.000       | .         |
| 1       | A     | 6   | VAL  | CG2  | 21.284     | 0.000       | .         |
| 1       | A     | 6   | VAL  | C    | 175.675    | 0.000       | .         |
| 1       | A     | 7   | ARG  | N    | 125.536    | 0.000       | .         |
| 1       | A     | 7   | ARG  | H    | 8.348      | 0.000       | .         |
| 1       | A     | 7   | ARG  | CA   | 53.951     | 0.000       | .         |
| 1       | A     | 7   | ARG  | HA   | 4.656      | 0.000       | .         |
| 1       | A     | 7   | ARG  | CB   | 30.577     | 0.000       | .         |
| 1       | A     | 7   | ARG  | HB2  | 1.758      | 0.000       | .         |
| 1       | A     | 7   | ARG  | HB3  | 1.928      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 7   | ARG  | CG   | 27.184     | 0.000       | .         |
| 1       | A     | 7   | ARG  | HG2  | 1.683      | 0.000       | .         |
| 1       | A     | 7   | ARG  | HG3  | 1.683      | 0.000       | .         |
| 1       | A     | 7   | ARG  | CD   | 43.35      | 0.000       | .         |
| 1       | A     | 7   | ARG  | HD2  | 3.247      | 0.000       | .         |
| 1       | A     | 7   | ARG  | HD3  | 3.247      | 0.000       | .         |
| 1       | A     | 7   | ARG  | C    | 173.819    | 0.000       | .         |
| 1       | A     | 8   | PRO  | CD   | 50.761     | 0.000       | .         |
| 1       | A     | 8   | PRO  | CA   | 63.053     | 0.000       | .         |
| 1       | A     | 8   | PRO  | HA   | 4.464      | 0.000       | .         |
| 1       | A     | 8   | PRO  | CB   | 31.987     | 0.000       | .         |
| 1       | A     | 8   | PRO  | HB2  | 2.209      | 0.000       | .         |
| 1       | A     | 8   | PRO  | HB3  | 2.209      | 0.000       | .         |
| 1       | A     | 8   | PRO  | CG   | 27.482     | 0.000       | .         |
| 1       | A     | 8   | PRO  | HG2  | 2.017      | 0.000       | .         |
| 1       | A     | 8   | PRO  | HG3  | 2.017      | 0.000       | .         |
| 1       | A     | 8   | PRO  | HD2  | 3.688      | 0.000       | .         |
| 1       | A     | 8   | PRO  | HD3  | 3.688      | 0.000       | .         |
| 1       | A     | 8   | PRO  | C    | 176.288    | 0.000       | .         |
| 1       | A     | 9   | ALA  | N    | 127.952    | 0.004       | .         |
| 1       | A     | 9   | ALA  | H    | 8.455      | 0.002       | .         |
| 1       | A     | 9   | ALA  | CA   | 50.229     | 0.000       | .         |
| 1       | A     | 9   | ALA  | HA   | 4.63       | 0.000       | .         |
| 1       | A     | 9   | ALA  | HB1  | 1.481      | 0.000       | .         |
| 1       | A     | 9   | ALA  | HB2  | 1.481      | 0.000       | .         |
| 1       | A     | 9   | ALA  | HB3  | 1.481      | 0.000       | .         |
| 1       | A     | 9   | ALA  | CB   | 18.177     | 0.000       | .         |
| 1       | A     | 9   | ALA  | C    | 174.697    | 0.000       | .         |
| 1       | A     | 10  | PRO  | CD   | 50.18      | 0.001       | .         |
| 1       | A     | 10  | PRO  | CA   | 63.786     | 0.001       | .         |
| 1       | A     | 10  | PRO  | HA   | 4.29       | 0.000       | .         |
| 1       | A     | 10  | PRO  | CB   | 31.684     | 0.000       | .         |
| 1       | A     | 10  | PRO  | HB2  | 2.591      | 0.000       | .         |
| 1       | A     | 10  | PRO  | HB3  | 2.591      | 0.000       | .         |
| 1       | A     | 10  | PRO  | CG   | 28.595     | 0.000       | .         |
| 1       | A     | 10  | PRO  | HG2  | 2.28       | 0.000       | .         |
| 1       | A     | 10  | PRO  | HG3  | 2.055      | 0.000       | .         |
| 1       | A     | 10  | PRO  | HD2  | 3.664      | 0.000       | .         |
| 1       | A     | 10  | PRO  | HD3  | 3.968      | 0.001       | .         |
| 1       | A     | 10  | PRO  | C    | 178.249    | 0.000       | .         |
| 1       | A     | 11  | GLY  | N    | 116.178    | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 11  | GLY  | H    | 9.682      | 0.000       | .         |
| 1       | A     | 11  | GLY  | CA   | 43.888     | 0.000       | .         |
| 1       | A     | 11  | GLY  | HA2  | 3.451      | 0.000       | .         |
| 1       | A     | 11  | GLY  | HA3  | 3.451      | 0.000       | .         |
| 1       | A     | 11  | GLY  | C    | 173.865    | 0.000       | .         |
| 1       | A     | 12  | GLU  | N    | 123.511    | 0.001       | .         |
| 1       | A     | 12  | GLU  | H    | 8.336      | 0.000       | .         |
| 1       | A     | 12  | GLU  | CA   | 55.292     | 0.000       | .         |
| 1       | A     | 12  | GLU  | HA   | 4.428      | 0.000       | .         |
| 1       | A     | 12  | GLU  | CB   | 31.489     | 0.001       | .         |
| 1       | A     | 12  | GLU  | HB2  | 2.153      | 0.000       | .         |
| 1       | A     | 12  | GLU  | HB3  | 2.285      | 0.000       | .         |
| 1       | A     | 12  | GLU  | CG   | 35.817     | 0.000       | .         |
| 1       | A     | 12  | GLU  | HG2  | 2.65       | 0.000       | .         |
| 1       | A     | 12  | GLU  | HG3  | 2.65       | 0.000       | .         |
| 1       | A     | 12  | GLU  | C    | 176.888    | 0.000       | .         |
| 1       | A     | 14  | THR  | N    | 122.262    | 0.000       | .         |
| 1       | A     | 14  | THR  | H    | 9.159      | 0.000       | .         |
| 1       | A     | 14  | THR  | CA   | 64.237     | 0.000       | .         |
| 1       | A     | 14  | THR  | HA   | 4.833      | 0.000       | .         |
| 1       | A     | 14  | THR  | CB   | 72.28      | 0.004       | .         |
| 1       | A     | 14  | THR  | HB   | 4.05       | 0.001       | .         |
| 1       | A     | 14  | THR  | HG21 | 1.476      | 0.000       | .         |
| 1       | A     | 14  | THR  | HG22 | 1.476      | 0.000       | .         |
| 1       | A     | 14  | THR  | HG23 | 1.476      | 0.000       | .         |
| 1       | A     | 14  | THR  | CG2  | 21.34      | 0.001       | .         |
| 1       | A     | 14  | THR  | C    | 171.334    | 0.000       | .         |
| 1       | A     | 15  | TRP  | N    | 121.304    | 0.000       | .         |
| 1       | A     | 15  | TRP  | H    | 7.928      | 0.000       | .         |
| 1       | A     | 15  | TRP  | CA   | 56.34      | 0.000       | .         |
| 1       | A     | 15  | TRP  | HA   | 4.6        | 0.000       | .         |
| 1       | A     | 15  | TRP  | CB   | 33.925     | 0.001       | .         |
| 1       | A     | 15  | TRP  | HB2  | 2.639      | 0.000       | .         |
| 1       | A     | 15  | TRP  | HB3  | 2.129      | 0.003       | .         |
| 1       | A     | 15  | TRP  | C    | 172.683    | 0.000       | .         |
| 1       | A     | 16  | VAL  | N    | 118.896    | 0.000       | .         |
| 1       | A     | 16  | VAL  | H    | 8.409      | 0.000       | .         |
| 1       | A     | 16  | VAL  | CA   | 58.355     | 0.000       | .         |
| 1       | A     | 16  | VAL  | HA   | 5.314      | 0.000       | .         |
| 1       | A     | 16  | VAL  | CB   | 34.946     | 0.000       | .         |
| 1       | A     | 16  | VAL  | HB   | 1.959      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 16  | VAL  | HG11 | -0.077     | 0.000       | .         |
| 1       | A     | 16  | VAL  | HG12 | -0.077     | 0.000       | .         |
| 1       | A     | 16  | VAL  | HG13 | -0.077     | 0.000       | .         |
| 1       | A     | 16  | VAL  | HG21 | 0.556      | 0.000       | .         |
| 1       | A     | 16  | VAL  | HG22 | 0.556      | 0.000       | .         |
| 1       | A     | 16  | VAL  | HG23 | 0.556      | 0.000       | .         |
| 1       | A     | 16  | VAL  | CG1  | 17.85      | 0.000       | .         |
| 1       | A     | 16  | VAL  | CG2  | 24.136     | 0.000       | .         |
| 1       | A     | 18  | LEU  | N    | 130.414    | 0.000       | .         |
| 1       | A     | 18  | LEU  | H    | 8.182      | 0.000       | .         |
| 1       | A     | 18  | LEU  | CA   | 52.747     | 0.000       | .         |
| 1       | A     | 18  | LEU  | HA   | 4.262      | 0.000       | .         |
| 1       | A     | 18  | LEU  | CB   | 40.951     | 0.006       | .         |
| 1       | A     | 18  | LEU  | HB2  | -1.652     | 0.000       | .         |
| 1       | A     | 18  | LEU  | HB3  | -0.96      | 0.000       | .         |
| 1       | A     | 18  | LEU  | CG   | 26.787     | 0.002       | .         |
| 1       | A     | 18  | LEU  | HG   | 0.649      | 0.000       | .         |
| 1       | A     | 18  | LEU  | HD11 | -0.1       | 0.000       | .         |
| 1       | A     | 18  | LEU  | HD12 | -0.1       | 0.000       | .         |
| 1       | A     | 18  | LEU  | HD13 | -0.1       | 0.000       | .         |
| 1       | A     | 18  | LEU  | HD21 | 0.371      | 0.001       | .         |
| 1       | A     | 18  | LEU  | HD22 | 0.371      | 0.001       | .         |
| 1       | A     | 18  | LEU  | HD23 | 0.371      | 0.001       | .         |
| 1       | A     | 18  | LEU  | CD1  | 22.315     | 0.000       | .         |
| 1       | A     | 18  | LEU  | CD2  | 25.602     | 0.000       | .         |
| 1       | A     | 18  | LEU  | C    | 173.802    | 0.000       | .         |
| 1       | A     | 19  | LEU  | N    | 124.941    | 0.000       | .         |
| 1       | A     | 19  | LEU  | H    | 7.217      | 0.004       | .         |
| 1       | A     | 19  | LEU  | CA   | 53.207     | 0.000       | .         |
| 1       | A     | 19  | LEU  | HA   | 4.826      | 0.000       | .         |
| 1       | A     | 19  | LEU  | CB   | 43.233     | 0.001       | .         |
| 1       | A     | 19  | LEU  | HB2  | 0.813      | 0.000       | .         |
| 1       | A     | 19  | LEU  | HB3  | 1.897      | 0.000       | .         |
| 1       | A     | 19  | LEU  | CG   | 26.129     | 0.000       | .         |
| 1       | A     | 19  | LEU  | HG   | 1.606      | 0.000       | .         |
| 1       | A     | 19  | LEU  | HD11 | 0.659      | 0.000       | .         |
| 1       | A     | 19  | LEU  | HD12 | 0.659      | 0.000       | .         |
| 1       | A     | 19  | LEU  | HD13 | 0.659      | 0.000       | .         |
| 1       | A     | 19  | LEU  | HD21 | 0.845      | 0.000       | .         |
| 1       | A     | 19  | LEU  | HD22 | 0.845      | 0.000       | .         |
| 1       | A     | 19  | LEU  | HD23 | 0.845      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 19  | LEU  | CD1  | 23.84      | 0.003       | .         |
| 1       | A     | 19  | LEU  | CD2  | 26.169     | 0.000       | .         |
| 1       | A     | 19  | LEU  | C    | 175.962    | 0.005       | .         |
| 1       | A     | 20  | THR  | N    | 117.663    | 0.000       | .         |
| 1       | A     | 20  | THR  | H    | 8.394      | 0.000       | .         |
| 1       | A     | 20  | THR  | CA   | 55.202     | 0.000       | .         |
| 1       | A     | 20  | THR  | HA   | 5.319      | 0.002       | .         |
| 1       | A     | 20  | THR  | CB   | 69.828     | 0.000       | .         |
| 1       | A     | 20  | THR  | HB   | 3.781      | 0.000       | .         |
| 1       | A     | 20  | THR  | HG21 | 0.981      | 0.000       | .         |
| 1       | A     | 20  | THR  | HG22 | 0.981      | 0.000       | .         |
| 1       | A     | 20  | THR  | HG23 | 0.981      | 0.000       | .         |
| 1       | A     | 20  | THR  | CG2  | 19.055     | 0.000       | .         |
| 1       | A     | 21  | PRO  | CD   | 52.418     | 0.000       | .         |
| 1       | A     | 21  | PRO  | CA   | 63.741     | 0.000       | .         |
| 1       | A     | 21  | PRO  | HA   | 4.803      | 0.001       | .         |
| 1       | A     | 21  | PRO  | CB   | 32.204     | 0.001       | .         |
| 1       | A     | 21  | PRO  | HB2  | 2.064      | 0.000       | .         |
| 1       | A     | 21  | PRO  | HB3  | 2.33       | 0.001       | .         |
| 1       | A     | 21  | PRO  | CG   | 26.639     | 0.002       | .         |
| 1       | A     | 21  | PRO  | HG2  | 2.064      | 0.000       | .         |
| 1       | A     | 21  | PRO  | HG3  | 2.064      | 0.000       | .         |
| 1       | A     | 21  | PRO  | HD2  | 3.692      | 0.000       | .         |
| 1       | A     | 21  | PRO  | HD3  | 4.157      | 0.001       | .         |
| 1       | A     | 21  | PRO  | C    | 175.371    | 0.000       | .         |
| 1       | A     | 22  | ASP  | N    | 119.544    | 0.000       | .         |
| 1       | A     | 22  | ASP  | H    | 8.117      | 0.000       | .         |
| 1       | A     | 22  | ASP  | CA   | 52.41      | 0.000       | .         |
| 1       | A     | 22  | ASP  | HA   | 4.863      | 0.000       | .         |
| 1       | A     | 22  | ASP  | CB   | 40.808     | 0.000       | .         |
| 1       | A     | 22  | ASP  | HB2  | 2.322      | 0.001       | .         |
| 1       | A     | 22  | ASP  | HB3  | 2.836      | 0.002       | .         |
| 1       | A     | 22  | ASP  | C    | 175.17     | 0.000       | .         |
| 1       | A     | 23  | ARG  | N    | 127.795    | 0.000       | .         |
| 1       | A     | 23  | ARG  | H    | 9.074      | 0.000       | .         |
| 1       | A     | 23  | ARG  | CA   | 60.065     | 0.000       | .         |
| 1       | A     | 23  | ARG  | HA   | 3.723      | 0.000       | .         |
| 1       | A     | 23  | ARG  | CB   | 30.82      | 0.000       | .         |
| 1       | A     | 23  | ARG  | HB2  | 1.925      | 0.000       | .         |
| 1       | A     | 23  | ARG  | HB3  | 1.627      | 0.000       | .         |
| 1       | A     | 23  | ARG  | CG   | 26.652     | 0.000       | .         |

*Continued on next page...*



*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 23  | ARG  | HG2  | 1.199      | 0.000       | .         |
| 1       | A     | 23  | ARG  | HG3  | 1.421      | 0.001       | .         |
| 1       | A     | 23  | ARG  | CD   | 44.39      | 0.001       | .         |
| 1       | A     | 23  | ARG  | HD2  | 2.639      | 0.000       | .         |
| 1       | A     | 23  | ARG  | HD3  | 3.219      | 0.001       | .         |
| 1       | A     | 23  | ARG  | C    | 177.08     | 0.000       | .         |
| 1       | A     | 24  | GLY  | N    | 106.757    | 0.000       | .         |
| 1       | A     | 24  | GLY  | H    | 8.928      | 0.000       | .         |
| 1       | A     | 24  | GLY  | CA   | 47.63      | 0.001       | .         |
| 1       | A     | 24  | GLY  | HA2  | 3.605      | 0.003       | .         |
| 1       | A     | 24  | GLY  | HA3  | 3.924      | 0.000       | .         |
| 1       | A     | 24  | GLY  | C    | 176.839    | 0.000       | .         |
| 1       | A     | 25  | ALA  | N    | 123.627    | 0.001       | .         |
| 1       | A     | 25  | ALA  | H    | 7.673      | 0.000       | .         |
| 1       | A     | 25  | ALA  | CA   | 54.372     | 0.000       | .         |
| 1       | A     | 25  | ALA  | HA   | 4.187      | 0.000       | .         |
| 1       | A     | 25  | ALA  | HB1  | 1.34       | 0.000       | .         |
| 1       | A     | 25  | ALA  | HB2  | 1.34       | 0.000       | .         |
| 1       | A     | 25  | ALA  | HB3  | 1.34       | 0.000       | .         |
| 1       | A     | 25  | ALA  | CB   | 18.564     | 0.000       | .         |
| 1       | A     | 25  | ALA  | C    | 181.046    | 0.000       | .         |
| 1       | A     | 26  | ALA  | N    | 123.192    | 0.000       | .         |
| 1       | A     | 26  | ALA  | H    | 7.885      | 0.000       | .         |
| 1       | A     | 26  | ALA  | CA   | 55.447     | 0.000       | .         |
| 1       | A     | 26  | ALA  | HA   | 4.342      | 0.000       | .         |
| 1       | A     | 26  | ALA  | HB1  | 1.662      | 0.000       | .         |
| 1       | A     | 26  | ALA  | HB2  | 1.662      | 0.000       | .         |
| 1       | A     | 26  | ALA  | HB3  | 1.662      | 0.000       | .         |
| 1       | A     | 26  | ALA  | CB   | 17.907     | 0.000       | .         |
| 1       | A     | 26  | ALA  | C    | 179.291    | 0.000       | .         |
| 1       | A     | 27  | LEU  | N    | 117.307    | 0.000       | .         |
| 1       | A     | 27  | LEU  | H    | 8.729      | 0.000       | .         |
| 1       | A     | 27  | LEU  | CA   | 58.367     | 0.001       | .         |
| 1       | A     | 27  | LEU  | HA   | 3.783      | 0.000       | .         |
| 1       | A     | 27  | LEU  | CB   | 39.284     | 0.000       | .         |
| 1       | A     | 27  | LEU  | HB2  | 1.105      | 0.000       | .         |
| 1       | A     | 27  | LEU  | HB3  | 1.643      | 0.000       | .         |
| 1       | A     | 27  | LEU  | CG   | 25.807     | 0.000       | .         |
| 1       | A     | 27  | LEU  | HG   | 1.486      | 0.000       | .         |
| 1       | A     | 27  | LEU  | HD11 | 0.043      | 0.000       | .         |
| 1       | A     | 27  | LEU  | HD12 | 0.043      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 27  | LEU  | HD13 | 0.043      | 0.000       | .         |
| 1       | A     | 27  | LEU  | HD21 | 0.483      | 0.000       | .         |
| 1       | A     | 27  | LEU  | HD22 | 0.483      | 0.000       | .         |
| 1       | A     | 27  | LEU  | HD23 | 0.483      | 0.000       | .         |
| 1       | A     | 27  | LEU  | CD1  | 22.051     | 0.000       | .         |
| 1       | A     | 27  | LEU  | CD2  | 24.415     | 0.000       | .         |
| 1       | A     | 27  | LEU  | C    | 180.064    | 0.008       | .         |
| 1       | A     | 28  | GLN  | N    | 116.385    | 0.001       | .         |
| 1       | A     | 28  | GLN  | H    | 7.249      | 0.000       | .         |
| 1       | A     | 28  | GLN  | CA   | 59.239     | 0.000       | .         |
| 1       | A     | 28  | GLN  | HA   | 4.03       | 0.000       | .         |
| 1       | A     | 28  | GLN  | CB   | 28.705     | 0.000       | .         |
| 1       | A     | 28  | GLN  | HB2  | 2.205      | 0.000       | .         |
| 1       | A     | 28  | GLN  | HB3  | 2.205      | 0.000       | .         |
| 1       | A     | 28  | GLN  | CG   | 33.918     | 0.002       | .         |
| 1       | A     | 28  | GLN  | HG2  | 2.442      | 0.000       | .         |
| 1       | A     | 28  | GLN  | HG3  | 2.553      | 0.000       | .         |
| 1       | A     | 28  | GLN  | NE2  | 111.986    | 0.001       | .         |
| 1       | A     | 28  | GLN  | HE21 | 6.842      | 0.000       | .         |
| 1       | A     | 28  | GLN  | HE22 | 7.469      | 0.000       | .         |
| 1       | A     | 28  | GLN  | C    | 177.913    | 0.000       | .         |
| 1       | A     | 29  | PHE  | N    | 120.866    | 0.001       | .         |
| 1       | A     | 29  | PHE  | H    | 7.699      | 0.000       | .         |
| 1       | A     | 29  | PHE  | CA   | 61.602     | 0.001       | .         |
| 1       | A     | 29  | PHE  | HA   | 4.16       | 0.000       | .         |
| 1       | A     | 29  | PHE  | CB   | 39.247     | 0.000       | .         |
| 1       | A     | 29  | PHE  | HB2  | 2.897      | 0.000       | .         |
| 1       | A     | 29  | PHE  | HB3  | 3.185      | 0.002       | .         |
| 1       | A     | 29  | PHE  | HD1  | 6.298      | 0.000       | .         |
| 1       | A     | 29  | PHE  | HD2  | 6.298      | 0.000       | .         |
| 1       | A     | 29  | PHE  | HE1  | 7.021      | 0.000       | .         |
| 1       | A     | 29  | PHE  | HE2  | 7.021      | 0.000       | .         |
| 1       | A     | 29  | PHE  | CD1  | 132.466    | 0.000       | .         |
| 1       | A     | 29  | PHE  | CE1  | 130.932    | 0.000       | .         |
| 1       | A     | 29  | PHE  | CZ   | 129.466    | 0.001       | .         |
| 1       | A     | 29  | PHE  | HZ   | 7.423      | 0.000       | .         |
| 1       | A     | 29  | PHE  | CE2  | 130.932    | 0.000       | .         |
| 1       | A     | 29  | PHE  | CD2  | 132.466    | 0.000       | .         |
| 1       | A     | 29  | PHE  | C    | 175.685    | 0.000       | .         |
| 1       | A     | 30  | TYR  | N    | 115.423    | 0.000       | .         |
| 1       | A     | 30  | TYR  | H    | 8.764      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 30  | TYR  | CA   | 63.628     | 0.000       | .         |
| 1       | A     | 30  | TYR  | HA   | 3.329      | 0.000       | .         |
| 1       | A     | 30  | TYR  | CB   | 39.219     | 0.000       | .         |
| 1       | A     | 30  | TYR  | HB2  | 2.676      | 0.000       | .         |
| 1       | A     | 30  | TYR  | HB3  | 2.911      | 0.000       | .         |
| 1       | A     | 30  | TYR  | HD1  | 6.19       | 0.000       | .         |
| 1       | A     | 30  | TYR  | HD2  | 6.19       | 0.000       | .         |
| 1       | A     | 30  | TYR  | HH   | 12.3       | 0.000       | .         |
| 1       | A     | 30  | TYR  | C    | 179.327    | 0.000       | .         |
| 1       | A     | 31  | SER  | N    | 113.142    | 0.000       | .         |
| 1       | A     | 31  | SER  | H    | 8.429      | 0.000       | .         |
| 1       | A     | 31  | SER  | CA   | 61.595     | 0.000       | .         |
| 1       | A     | 31  | SER  | HA   | 4.092      | 0.000       | .         |
| 1       | A     | 31  | SER  | CB   | 63.023     | 0.000       | .         |
| 1       | A     | 31  | SER  | HB2  | 4.231      | 0.000       | .         |
| 1       | A     | 31  | SER  | HB3  | 4.303      | 0.000       | .         |
| 1       | A     | 31  | SER  | C    | 177.549    | 0.000       | .         |
| 1       | A     | 32  | ALA  | N    | 124.159    | 0.000       | .         |
| 1       | A     | 32  | ALA  | H    | 7.296      | 0.000       | .         |
| 1       | A     | 32  | ALA  | CA   | 54.808     | 0.000       | .         |
| 1       | A     | 32  | ALA  | HA   | 3.983      | 0.000       | .         |
| 1       | A     | 32  | ALA  | HB1  | 1.388      | 0.000       | .         |
| 1       | A     | 32  | ALA  | HB2  | 1.388      | 0.000       | .         |
| 1       | A     | 32  | ALA  | HB3  | 1.388      | 0.000       | .         |
| 1       | A     | 32  | ALA  | CB   | 18.512     | 0.000       | .         |
| 1       | A     | 32  | ALA  | C    | 179.317    | 0.000       | .         |
| 1       | A     | 33  | LEU  | N    | 116.441    | 0.000       | .         |
| 1       | A     | 33  | LEU  | H    | 7.423      | 0.000       | .         |
| 1       | A     | 33  | LEU  | CA   | 56.722     | 0.000       | .         |
| 1       | A     | 33  | LEU  | HA   | 3.606      | 0.000       | .         |
| 1       | A     | 33  | LEU  | CB   | 42.451     | 0.000       | .         |
| 1       | A     | 33  | LEU  | HB2  | 0.114      | 0.000       | .         |
| 1       | A     | 33  | LEU  | HB3  | 0.198      | 0.000       | .         |
| 1       | A     | 33  | LEU  | CG   | 25.9       | 0.000       | .         |
| 1       | A     | 33  | LEU  | HG   | 0.191      | 0.000       | .         |
| 1       | A     | 33  | LEU  | HD11 | 0.362      | 0.000       | .         |
| 1       | A     | 33  | LEU  | HD12 | 0.362      | 0.000       | .         |
| 1       | A     | 33  | LEU  | HD13 | 0.362      | 0.000       | .         |
| 1       | A     | 33  | LEU  | HD21 | 0.106      | 0.000       | .         |
| 1       | A     | 33  | LEU  | HD22 | 0.106      | 0.000       | .         |
| 1       | A     | 33  | LEU  | HD23 | 0.106      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 33  | LEU  | CD1  | 23.513     | 0.000       | .         |
| 1       | A     | 33  | LEU  | CD2  | 26.209     | 0.000       | .         |
| 1       | A     | 33  | LEU  | C    | 177.539    | 0.000       | .         |
| 1       | A     | 34  | PHE  | N    | 111.581    | 0.001       | .         |
| 1       | A     | 34  | PHE  | H    | 7.45       | 0.000       | .         |
| 1       | A     | 34  | PHE  | CA   | 55.796     | 0.000       | .         |
| 1       | A     | 34  | PHE  | HA   | 4.761      | 0.000       | .         |
| 1       | A     | 34  | PHE  | CB   | 41.298     | 0.000       | .         |
| 1       | A     | 34  | PHE  | HB2  | 1.153      | 0.000       | .         |
| 1       | A     | 34  | PHE  | HB3  | 2.723      | 0.000       | .         |
| 1       | A     | 34  | PHE  | HD1  | 6.129      | 0.000       | .         |
| 1       | A     | 34  | PHE  | HD2  | 6.129      | 0.000       | .         |
| 1       | A     | 34  | PHE  | HE1  | 6.476      | 0.000       | .         |
| 1       | A     | 34  | PHE  | HE2  | 6.476      | 0.000       | .         |
| 1       | A     | 34  | PHE  | CD1  | 130.824    | 0.000       | .         |
| 1       | A     | 34  | PHE  | CE1  | 129.585    | 0.000       | .         |
| 1       | A     | 34  | PHE  | CZ   | 129.397    | 0.006       | .         |
| 1       | A     | 34  | PHE  | HZ   | 6.897      | 0.003       | .         |
| 1       | A     | 34  | PHE  | CE2  | 129.585    | 0.000       | .         |
| 1       | A     | 34  | PHE  | CD2  | 130.824    | 0.000       | .         |
| 1       | A     | 34  | PHE  | C    | 176.881    | 0.000       | .         |
| 1       | A     | 35  | GLY  | N    | 107.358    | 0.001       | .         |
| 1       | A     | 35  | GLY  | H    | 7.97       | 0.000       | .         |
| 1       | A     | 35  | GLY  | CA   | 45.825     | 0.000       | .         |
| 1       | A     | 35  | GLY  | HA2  | 3.944      | 0.000       | .         |
| 1       | A     | 35  | GLY  | HA3  | 4.095      | 0.000       | .         |
| 1       | A     | 35  | GLY  | C    | 174.241    | 0.000       | .         |
| 1       | A     | 36  | TRP  | N    | 116.638    | 0.000       | .         |
| 1       | A     | 36  | TRP  | H    | 6.177      | 0.000       | .         |
| 1       | A     | 36  | TRP  | CA   | 55.387     | 0.000       | .         |
| 1       | A     | 36  | TRP  | HA   | 4.732      | 0.000       | .         |
| 1       | A     | 36  | TRP  | CB   | 30.984     | 0.000       | .         |
| 1       | A     | 36  | TRP  | HB2  | 2.752      | 0.000       | .         |
| 1       | A     | 36  | TRP  | HB3  | 2.772      | 0.000       | .         |
| 1       | A     | 36  | TRP  | CD1  | 122.774    | 0.000       | .         |
| 1       | A     | 36  | TRP  | CE3  | 119.7      | 0.000       | .         |
| 1       | A     | 36  | TRP  | NE1  | 129.181    | 0.000       | .         |
| 1       | A     | 36  | TRP  | HD1  | 6.714      | 0.000       | .         |
| 1       | A     | 36  | TRP  | HE3  | 7.312      | 0.000       | .         |
| 1       | A     | 36  | TRP  | CZ3  | 121.81     | 0.005       | .         |
| 1       | A     | 36  | TRP  | CZ2  | 115.722    | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 36  | TRP  | HE1  | 10.46      | 0.000       | .         |
| 1       | A     | 36  | TRP  | HZ3  | 6.341      | 0.002       | .         |
| 1       | A     | 36  | TRP  | CH2  | 125.482    | 0.001       | .         |
| 1       | A     | 36  | TRP  | HZ2  | 5.912      | 0.000       | .         |
| 1       | A     | 36  | TRP  | HH2  | 5.856      | 0.003       | .         |
| 1       | A     | 36  | TRP  | C    | 173.96     | 0.000       | .         |
| 1       | A     | 37  | GLU  | N    | 119.397    | 0.000       | .         |
| 1       | A     | 37  | GLU  | H    | 9.109      | 0.000       | .         |
| 1       | A     | 37  | GLU  | CA   | 54.174     | 0.001       | .         |
| 1       | A     | 37  | GLU  | HA   | 4.148      | 0.000       | .         |
| 1       | A     | 37  | GLU  | CB   | 32.445     | 0.000       | .         |
| 1       | A     | 37  | GLU  | HB2  | 1.792      | 0.001       | .         |
| 1       | A     | 37  | GLU  | HB3  | 1.943      | 0.000       | .         |
| 1       | A     | 37  | GLU  | CG   | 36.62      | 0.003       | .         |
| 1       | A     | 37  | GLU  | HG2  | 2.139      | 0.000       | .         |
| 1       | A     | 37  | GLU  | HG3  | 2.31       | 0.000       | .         |
| 1       | A     | 37  | GLU  | C    | 176.001    | 0.003       | .         |
| 1       | A     | 38  | PHE  | N    | 120.741    | 0.000       | .         |
| 1       | A     | 38  | PHE  | H    | 8.491      | 0.000       | .         |
| 1       | A     | 38  | PHE  | CA   | 55.995     | 0.002       | .         |
| 1       | A     | 38  | PHE  | HA   | 5.712      | 0.000       | .         |
| 1       | A     | 38  | PHE  | CB   | 41.996     | 0.001       | .         |
| 1       | A     | 38  | PHE  | HB2  | 2.891      | 0.000       | .         |
| 1       | A     | 38  | PHE  | HB3  | 3.241      | 0.000       | .         |
| 1       | A     | 38  | PHE  | HD1  | 7.27       | 0.000       | .         |
| 1       | A     | 38  | PHE  | HD2  | 7.27       | 0.000       | .         |
| 1       | A     | 38  | PHE  | CD1  | 131.912    | 0.000       | .         |
| 1       | A     | 38  | PHE  | CD2  | 131.912    | 0.002       | .         |
| 1       | A     | 38  | PHE  | C    | 176.294    | 0.000       | .         |
| 1       | A     | 39  | SER  | N    | 117.062    | 0.000       | .         |
| 1       | A     | 39  | SER  | H    | 8.879      | 0.000       | .         |
| 1       | A     | 39  | SER  | CA   | 57.323     | 0.000       | .         |
| 1       | A     | 39  | SER  | HA   | 4.814      | 0.000       | .         |
| 1       | A     | 39  | SER  | CB   | 65.143     | 0.000       | .         |
| 1       | A     | 39  | SER  | HB2  | 3.831      | 0.000       | .         |
| 1       | A     | 39  | SER  | HB3  | 3.831      | 0.000       | .         |
| 1       | A     | 39  | SER  | C    | 173.603    | 0.000       | .         |
| 1       | A     | 40  | THR  | N    | 122.348    | 0.000       | .         |
| 1       | A     | 40  | THR  | H    | 8.892      | 0.000       | .         |
| 1       | A     | 40  | THR  | CA   | 62.89      | 0.001       | .         |
| 1       | A     | 40  | THR  | HA   | 4.721      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 40  | THR  | CB   | 69.362     | 0.005       | .         |
| 1       | A     | 40  | THR  | HB   | 4.083      | 0.000       | .         |
| 1       | A     | 40  | THR  | HG21 | 1.239      | 0.000       | .         |
| 1       | A     | 40  | THR  | HG22 | 1.239      | 0.000       | .         |
| 1       | A     | 40  | THR  | HG23 | 1.239      | 0.000       | .         |
| 1       | A     | 40  | THR  | CG2  | 21.873     | 0.000       | .         |
| 1       | A     | 41  | THR  | N    | 123.272    | 0.000       | .         |
| 1       | A     | 41  | THR  | H    | 8.796      | 0.000       | .         |
| 1       | A     | 41  | THR  | CA   | 60.24      | 0.000       | .         |
| 1       | A     | 41  | THR  | HA   | 4.491      | 0.000       | .         |
| 1       | A     | 41  | THR  | CB   | 69.724     | 0.001       | .         |
| 1       | A     | 41  | THR  | HB   | 3.682      | 0.001       | .         |
| 1       | A     | 41  | THR  | HG21 | 0.733      | 0.000       | .         |
| 1       | A     | 41  | THR  | HG22 | 0.733      | 0.000       | .         |
| 1       | A     | 41  | THR  | HG23 | 0.733      | 0.000       | .         |
| 1       | A     | 41  | THR  | CG2  | 21.619     | 0.000       | .         |
| 1       | A     | 41  | THR  | C    | 172.696    | 0.000       | .         |
| 1       | A     | 43  | ASP  | N    | 123.551    | 0.000       | .         |
| 1       | A     | 43  | ASP  | H    | 8.579      | 0.000       | .         |
| 1       | A     | 43  | ASP  | CA   | 54.126     | 0.000       | .         |
| 1       | A     | 43  | ASP  | HA   | 4.868      | 0.000       | .         |
| 1       | A     | 43  | ASP  | CB   | 41.328     | 0.002       | .         |
| 1       | A     | 43  | ASP  | HB2  | 2.904      | 0.000       | .         |
| 1       | A     | 43  | ASP  | HB3  | 2.737      | 0.001       | .         |
| 1       | A     | 43  | ASP  | C    | 176.289    | 0.000       | .         |
| 1       | A     | 44  | GLY  | N    | 109.288    | 0.000       | .         |
| 1       | A     | 44  | GLY  | H    | 8.697      | 0.000       | .         |
| 1       | A     | 44  | GLY  | CA   | 45.353     | 0.003       | .         |
| 1       | A     | 44  | GLY  | HA2  | 3.835      | 0.000       | .         |
| 1       | A     | 44  | GLY  | HA3  | 4.369      | 0.000       | .         |
| 1       | A     | 44  | GLY  | C    | 174.513    | 0.006       | .         |
| 1       | A     | 45  | THR  | N    | 114.17     | 0.000       | .         |
| 1       | A     | 45  | THR  | H    | 8.375      | 0.000       | .         |
| 1       | A     | 45  | THR  | CA   | 63.078     | 0.000       | .         |
| 1       | A     | 45  | THR  | HA   | 4.443      | 0.000       | .         |
| 1       | A     | 45  | THR  | CB   | 70.499     | 0.001       | .         |
| 1       | A     | 45  | THR  | HB   | 4.358      | 0.000       | .         |
| 1       | A     | 45  | THR  | HG21 | 1.263      | 0.000       | .         |
| 1       | A     | 45  | THR  | HG22 | 1.263      | 0.000       | .         |
| 1       | A     | 45  | THR  | HG23 | 1.263      | 0.000       | .         |
| 1       | A     | 45  | THR  | CG2  | 21.675     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 46  | SER  | CA   | 55.881     | 0.000       | .         |
| 1       | A     | 46  | SER  | HA   | 4.875      | 0.000       | .         |
| 1       | A     | 46  | SER  | CB   | 64.2       | 0.000       | .         |
| 1       | A     | 46  | SER  | HB2  | 3.861      | 0.000       | .         |
| 1       | A     | 46  | SER  | HB3  | 3.861      | 0.000       | .         |
| 1       | A     | 48  | TYR  | CA   | 56.442     | 0.000       | .         |
| 1       | A     | 48  | TYR  | HA   | 4.794      | 0.000       | .         |
| 1       | A     | 48  | TYR  | CB   | 39.358     | 0.001       | .         |
| 1       | A     | 48  | TYR  | HB2  | 3.159      | 0.000       | .         |
| 1       | A     | 48  | TYR  | HB3  | 3.159      | 0.000       | .         |
| 1       | A     | 48  | TYR  | HD1  | 7.062      | 0.001       | .         |
| 1       | A     | 48  | TYR  | HD2  | 7.062      | 0.001       | .         |
| 1       | A     | 48  | TYR  | HE1  | 6.692      | 0.004       | .         |
| 1       | A     | 48  | TYR  | HE2  | 6.692      | 0.004       | .         |
| 1       | A     | 48  | TYR  | CD1  | 134.56     | 0.005       | .         |
| 1       | A     | 48  | TYR  | CE1  | 118.176    | 0.007       | .         |
| 1       | A     | 48  | TYR  | CE2  | 118.176    | 0.000       | .         |
| 1       | A     | 48  | TYR  | CD2  | 134.56     | 0.000       | .         |
| 1       | A     | 49  | THR  | N    | 118.084    | 0.000       | .         |
| 1       | A     | 49  | THR  | H    | 9.447      | 0.000       | .         |
| 1       | A     | 49  | THR  | CA   | 63.309     | 0.001       | .         |
| 1       | A     | 49  | THR  | HA   | 4.678      | 0.000       | .         |
| 1       | A     | 49  | THR  | CB   | 71.62      | 0.001       | .         |
| 1       | A     | 49  | THR  | HB   | 4.049      | 0.000       | .         |
| 1       | A     | 49  | THR  | HG21 | 1.305      | 0.000       | .         |
| 1       | A     | 49  | THR  | HG22 | 1.305      | 0.000       | .         |
| 1       | A     | 49  | THR  | HG23 | 1.305      | 0.000       | .         |
| 1       | A     | 49  | THR  | CG2  | 23.706     | 0.008       | .         |
| 1       | A     | 50  | MET  | N    | 126.406    | 0.000       | .         |
| 1       | A     | 50  | MET  | H    | 9.006      | 0.000       | .         |
| 1       | A     | 50  | MET  | CA   | 53.625     | 0.001       | .         |
| 1       | A     | 50  | MET  | HA   | 5.062      | 0.002       | .         |
| 1       | A     | 50  | MET  | CB   | 33.455     | 0.000       | .         |
| 1       | A     | 50  | MET  | HB2  | 2.027      | 0.000       | .         |
| 1       | A     | 50  | MET  | HB3  | 2.027      | 0.000       | .         |
| 1       | A     | 50  | MET  | CG   | 32.5       | 0.001       | .         |
| 1       | A     | 50  | MET  | HG2  | 2.453      | 0.000       | .         |
| 1       | A     | 50  | MET  | HG3  | 2.731      | 0.000       | .         |
| 1       | A     | 50  | MET  | HE1  | 2.05       | 0.000       | .         |
| 1       | A     | 50  | MET  | HE2  | 2.05       | 0.000       | .         |
| 1       | A     | 50  | MET  | HE3  | 2.05       | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 50  | MET  | CE   | 16.962     | 0.000       | .         |
| 1       | A     | 50  | MET  | C    | 175.409    | 0.000       | .         |
| 1       | A     | 51  | CYS  | N    | 125.134    | 0.005       | .         |
| 1       | A     | 51  | CYS  | H    | 8.743      | 0.001       | .         |
| 1       | A     | 51  | CYS  | CA   | 56.817     | 0.000       | .         |
| 1       | A     | 51  | CYS  | HA   | 5.112      | 0.000       | .         |
| 1       | A     | 51  | CYS  | CB   | 28.266     | 0.003       | .         |
| 1       | A     | 51  | CYS  | HB2  | 1.904      | 0.000       | .         |
| 1       | A     | 51  | CYS  | HB3  | 2.607      | 0.000       | .         |
| 1       | A     | 51  | CYS  | C    | 174.058    | 0.004       | .         |
| 1       | A     | 52  | ARG  | N    | 123.912    | 0.001       | .         |
| 1       | A     | 52  | ARG  | H    | 9.473      | 0.000       | .         |
| 1       | A     | 52  | ARG  | CA   | 54.459     | 0.000       | .         |
| 1       | A     | 52  | ARG  | HA   | 5.278      | 0.000       | .         |
| 1       | A     | 52  | ARG  | CB   | 35.04      | 0.000       | .         |
| 1       | A     | 52  | ARG  | HB2  | 1.451      | 0.000       | .         |
| 1       | A     | 52  | ARG  | HB3  | 1.511      | 0.000       | .         |
| 1       | A     | 52  | ARG  | CG   | 28.193     | 0.000       | .         |
| 1       | A     | 52  | ARG  | HG2  | 1.307      | 0.000       | .         |
| 1       | A     | 52  | ARG  | HG3  | 1.407      | 0.000       | .         |
| 1       | A     | 52  | ARG  | CD   | 43.422     | 0.001       | .         |
| 1       | A     | 52  | ARG  | HD2  | 2.951      | 0.000       | .         |
| 1       | A     | 52  | ARG  | HD3  | 3.129      | 0.000       | .         |
| 1       | A     | 52  | ARG  | NE   | 84.14      | 0.000       | .         |
| 1       | A     | 52  | ARG  | HE   | 7.338      | 0.000       | .         |
| 1       | A     | 52  | ARG  | C    | 174.196    | 0.000       | .         |
| 1       | A     | 53  | LEU  | N    | 120.396    | 0.000       | .         |
| 1       | A     | 53  | LEU  | H    | 8.771      | 0.000       | .         |
| 1       | A     | 53  | LEU  | CA   | 54.666     | 0.000       | .         |
| 1       | A     | 53  | LEU  | HA   | 4.636      | 0.000       | .         |
| 1       | A     | 53  | LEU  | CB   | 45.926     | 0.000       | .         |
| 1       | A     | 53  | LEU  | HB2  | 1.365      | 0.000       | .         |
| 1       | A     | 53  | LEU  | HB3  | 1.606      | 0.000       | .         |
| 1       | A     | 53  | LEU  | CG   | 27.604     | 0.000       | .         |
| 1       | A     | 53  | LEU  | HG   | 1.291      | 0.000       | .         |
| 1       | A     | 53  | LEU  | HD11 | 1.122      | 0.000       | .         |
| 1       | A     | 53  | LEU  | HD12 | 1.122      | 0.000       | .         |
| 1       | A     | 53  | LEU  | HD13 | 1.122      | 0.000       | .         |
| 1       | A     | 53  | LEU  | HD21 | 1.085      | 0.000       | .         |
| 1       | A     | 53  | LEU  | HD22 | 1.085      | 0.000       | .         |
| 1       | A     | 53  | LEU  | HD23 | 1.085      | 0.000       | .         |

*Continued on next page...*



*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 53  | LEU  | CD1  | 22.928     | 0.000       | .         |
| 1       | A     | 53  | LEU  | CD2  | 26.406     | 0.000       | .         |
| 1       | A     | 53  | LEU  | C    | 176.473    | 0.004       | .         |
| 1       | A     | 54  | ARG  | N    | 126.897    | 0.000       | .         |
| 1       | A     | 54  | ARG  | H    | 9.74       | 0.000       | .         |
| 1       | A     | 54  | ARG  | CA   | 57.675     | 0.000       | .         |
| 1       | A     | 54  | ARG  | HA   | 3.871      | 0.000       | .         |
| 1       | A     | 54  | ARG  | CB   | 28.496     | 0.000       | .         |
| 1       | A     | 54  | ARG  | HB2  | 1.923      | 0.000       | .         |
| 1       | A     | 54  | ARG  | HB3  | 1.923      | 0.000       | .         |
| 1       | A     | 54  | ARG  | C    | 176.38     | 0.000       | .         |
| 1       | A     | 55  | GLY  | N    | 103.009    | 0.001       | .         |
| 1       | A     | 55  | GLY  | H    | 8.823      | 0.000       | .         |
| 1       | A     | 55  | GLY  | CA   | 45.428     | 0.000       | .         |
| 1       | A     | 55  | GLY  | HA2  | 3.601      | 0.001       | .         |
| 1       | A     | 55  | GLY  | HA3  | 4.174      | 0.000       | .         |
| 1       | A     | 55  | GLY  | C    | 174.135    | 0.000       | .         |
| 1       | A     | 56  | ARG  | N    | 119.717    | 0.000       | .         |
| 1       | A     | 56  | ARG  | H    | 7.794      | 0.000       | .         |
| 1       | A     | 56  | ARG  | CA   | 53.551     | 0.000       | .         |
| 1       | A     | 56  | ARG  | HA   | 4.749      | 0.000       | .         |
| 1       | A     | 56  | ARG  | CB   | 32.528     | 0.000       | .         |
| 1       | A     | 56  | ARG  | HB2  | 1.995      | 0.000       | .         |
| 1       | A     | 56  | ARG  | HB3  | 1.825      | 0.000       | .         |
| 1       | A     | 56  | ARG  | CG   | 27.373     | 0.001       | .         |
| 1       | A     | 56  | ARG  | HG2  | 1.701      | 0.001       | .         |
| 1       | A     | 56  | ARG  | HG3  | 1.701      | 0.001       | .         |
| 1       | A     | 56  | ARG  | CD   | 42.997     | 0.000       | .         |
| 1       | A     | 56  | ARG  | HD2  | 3.21       | 0.001       | .         |
| 1       | A     | 56  | ARG  | HD3  | 3.21       | 0.001       | .         |
| 1       | A     | 56  | ARG  | NE   | 85.286     | 0.000       | .         |
| 1       | A     | 56  | ARG  | HE   | 7.341      | 0.000       | .         |
| 1       | A     | 56  | ARG  | C    | 175.553    | 0.000       | .         |
| 1       | A     | 57  | GLU  | N    | 120.572    | 0.001       | .         |
| 1       | A     | 57  | GLU  | H    | 8.874      | 0.000       | .         |
| 1       | A     | 57  | GLU  | CA   | 57.226     | 0.000       | .         |
| 1       | A     | 57  | GLU  | HA   | 4.317      | 0.000       | .         |
| 1       | A     | 57  | GLU  | CB   | 29.895     | 0.000       | .         |
| 1       | A     | 57  | GLU  | HB2  | 2.212      | 0.000       | .         |
| 1       | A     | 57  | GLU  | HB3  | 2.212      | 0.000       | .         |
| 1       | A     | 57  | GLU  | C    | 175.672    | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 58  | VAL  | N    | 122.747    | 0.000       | .         |
| 1       | A     | 58  | VAL  | H    | 8.99       | 0.000       | .         |
| 1       | A     | 58  | VAL  | CA   | 63.673     | 0.000       | .         |
| 1       | A     | 58  | VAL  | HA   | 3.943      | 0.000       | .         |
| 1       | A     | 58  | VAL  | CB   | 34.455     | 0.000       | .         |
| 1       | A     | 58  | VAL  | HB   | 0.832      | 0.000       | .         |
| 1       | A     | 58  | VAL  | HG11 | 0.492      | 0.000       | .         |
| 1       | A     | 58  | VAL  | HG12 | 0.492      | 0.000       | .         |
| 1       | A     | 58  | VAL  | HG13 | 0.492      | 0.000       | .         |
| 1       | A     | 58  | VAL  | HG21 | 0.586      | 0.000       | .         |
| 1       | A     | 58  | VAL  | HG22 | 0.586      | 0.000       | .         |
| 1       | A     | 58  | VAL  | HG23 | 0.586      | 0.000       | .         |
| 1       | A     | 58  | VAL  | CG1  | 20.593     | 0.000       | .         |
| 1       | A     | 58  | VAL  | CG2  | 21.54      | 0.000       | .         |
| 1       | A     | 58  | VAL  | C    | 174.902    | 0.000       | .         |
| 1       | A     | 59  | CYS  | N    | 109.691    | 0.000       | .         |
| 1       | A     | 59  | CYS  | H    | 6.905      | 0.000       | .         |
| 1       | A     | 59  | CYS  | CA   | 56.121     | 0.000       | .         |
| 1       | A     | 59  | CYS  | HA   | 2.357      | 0.000       | .         |
| 1       | A     | 59  | CYS  | CB   | 28.554     | 0.000       | .         |
| 1       | A     | 59  | CYS  | HB2  | 2.745      | 0.000       | .         |
| 1       | A     | 59  | CYS  | HB3  | 2.211      | 0.000       | .         |
| 1       | A     | 59  | CYS  | C    | 170.685    | 0.000       | .         |
| 1       | A     | 60  | SER  | N    | 108.236    | 0.000       | .         |
| 1       | A     | 60  | SER  | H    | 7.254      | 0.000       | .         |
| 1       | A     | 60  | SER  | CA   | 56.623     | 0.000       | .         |
| 1       | A     | 60  | SER  | HA   | 5.564      | 0.000       | .         |
| 1       | A     | 60  | SER  | CB   | 66.289     | 0.002       | .         |
| 1       | A     | 60  | SER  | HB2  | 4.034      | 0.000       | .         |
| 1       | A     | 60  | SER  | HB3  | 4.089      | 0.000       | .         |
| 1       | A     | 61  | ILE  | N    | 117.918    | 0.000       | .         |
| 1       | A     | 61  | ILE  | H    | 8.836      | 0.000       | .         |
| 1       | A     | 61  | ILE  | CA   | 60.69      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HA   | 4.73       | 0.000       | .         |
| 1       | A     | 61  | ILE  | CB   | 42.335     | 0.002       | .         |
| 1       | A     | 61  | ILE  | HB   | 1.236      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HG21 | 0.628      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HG22 | 0.628      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HG23 | 0.628      | 0.000       | .         |
| 1       | A     | 61  | ILE  | CG2  | 17.202     | 0.000       | .         |
| 1       | A     | 61  | ILE  | CG1  | 26.934     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 61  | ILE  | HG12 | 1.439      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HG13 | 1.439      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HD11 | 0.725      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HD12 | 0.725      | 0.000       | .         |
| 1       | A     | 61  | ILE  | HD13 | 0.725      | 0.000       | .         |
| 1       | A     | 61  | ILE  | CD1  | 14.265     | 0.005       | .         |
| 1       | A     | 61  | ILE  | C    | 174.227    | 0.000       | .         |
| 1       | A     | 62  | GLY  | N    | 115.062    | 0.000       | .         |
| 1       | A     | 62  | GLY  | H    | 9.563      | 0.000       | .         |
| 1       | A     | 62  | GLY  | CA   | 43.994     | 0.000       | .         |
| 1       | A     | 62  | GLY  | HA2  | 3.982      | 0.000       | .         |
| 1       | A     | 62  | GLY  | HA3  | 3.982      | 0.000       | .         |
| 1       | A     | 63  | ASP  | CA   | 54.092     | 0.000       | .         |
| 1       | A     | 63  | ASP  | HA   | 4.96       | 0.007       | .         |
| 1       | A     | 63  | ASP  | CB   | 41.514     | 0.001       | .         |
| 1       | A     | 63  | ASP  | HB2  | 2.569      | 0.000       | .         |
| 1       | A     | 63  | ASP  | HB3  | 2.73       | 0.000       | .         |
| 1       | A     | 63  | ASP  | C    | 175.806    | 0.000       | .         |
| 1       | A     | 64  | LEU  | N    | 124.619    | 0.000       | .         |
| 1       | A     | 64  | LEU  | H    | 7.635      | 0.000       | .         |
| 1       | A     | 64  | LEU  | CA   | 55.946     | 0.000       | .         |
| 1       | A     | 64  | LEU  | HA   | 4.055      | 0.000       | .         |
| 1       | A     | 64  | LEU  | CB   | 43.459     | 0.001       | .         |
| 1       | A     | 64  | LEU  | HB2  | 0.827      | 0.002       | .         |
| 1       | A     | 64  | LEU  | HB3  | 1.484      | 0.000       | .         |
| 1       | A     | 64  | LEU  | CG   | 26.299     | 0.001       | .         |
| 1       | A     | 64  | LEU  | HG   | 0.83       | 0.000       | .         |
| 1       | A     | 64  | LEU  | HD11 | 0.721      | 0.000       | .         |
| 1       | A     | 64  | LEU  | HD12 | 0.721      | 0.000       | .         |
| 1       | A     | 64  | LEU  | HD13 | 0.721      | 0.000       | .         |
| 1       | A     | 64  | LEU  | HD21 | 0.826      | 0.000       | .         |
| 1       | A     | 64  | LEU  | HD22 | 0.826      | 0.000       | .         |
| 1       | A     | 64  | LEU  | HD23 | 0.826      | 0.000       | .         |
| 1       | A     | 64  | LEU  | CD1  | 23.912     | 0.000       | .         |
| 1       | A     | 64  | LEU  | CD2  | 25.945     | 0.000       | .         |
| 1       | A     | 64  | LEU  | C    | 176.877    | 0.002       | .         |
| 1       | A     | 66  | GLU  | CA   | 56.365     | 0.000       | .         |
| 1       | A     | 66  | GLU  | HA   | 4.282      | 0.000       | .         |
| 1       | A     | 66  | GLU  | CB   | 30.032     | 0.000       | .         |
| 1       | A     | 66  | GLU  | HB2  | 1.873      | 0.000       | .         |
| 1       | A     | 66  | GLU  | HB3  | 2.108      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 66  | GLU  | CG   | 36.307     | 0.001       | .         |
| 1       | A     | 66  | GLU  | HG2  | 2.275      | 0.000       | .         |
| 1       | A     | 66  | GLU  | HG3  | 2.213      | 0.000       | .         |
| 1       | A     | 66  | GLU  | C    | 176.388    | 0.000       | .         |
| 1       | A     | 67  | ASN  | N    | 118.803    | 0.000       | .         |
| 1       | A     | 67  | ASN  | H    | 8.291      | 0.000       | .         |
| 1       | A     | 67  | ASN  | CA   | 51.983     | 0.001       | .         |
| 1       | A     | 67  | ASN  | HA   | 4.867      | 0.000       | .         |
| 1       | A     | 67  | ASN  | CB   | 39.192     | 0.002       | .         |
| 1       | A     | 67  | ASN  | HB2  | 2.653      | 0.000       | .         |
| 1       | A     | 67  | ASN  | HB3  | 2.654      | 0.001       | .         |
| 1       | A     | 67  | ASN  | ND2  | 114.317    | 0.000       | .         |
| 1       | A     | 67  | ASN  | HD21 | 6.879      | 0.000       | .         |
| 1       | A     | 67  | ASN  | HD22 | 7.593      | 0.000       | .         |
| 1       | A     | 67  | ASN  | C    | 172.678    | 0.000       | .         |
| 1       | A     | 68  | PRO  | CD   | 50.406     | 0.000       | .         |
| 1       | A     | 68  | PRO  | CA   | 63.915     | 0.005       | .         |
| 1       | A     | 68  | PRO  | HA   | 4.43       | 0.000       | .         |
| 1       | A     | 68  | PRO  | CB   | 32.232     | 0.000       | .         |
| 1       | A     | 68  | PRO  | HB2  | 2.012      | 0.000       | .         |
| 1       | A     | 68  | PRO  | HB3  | 2.193      | 0.000       | .         |
| 1       | A     | 68  | PRO  | CG   | 27.152     | 0.003       | .         |
| 1       | A     | 68  | PRO  | HG2  | 1.963      | 0.000       | .         |
| 1       | A     | 68  | PRO  | HG3  | 2.036      | 0.000       | .         |
| 1       | A     | 68  | PRO  | HD2  | 3.676      | 0.000       | .         |
| 1       | A     | 68  | PRO  | HD3  | 3.676      | 0.000       | .         |
| 1       | A     | 68  | PRO  | C    | 176.33     | 0.000       | .         |
| 1       | A     | 69  | GLY  | N    | 111.249    | 0.000       | .         |
| 1       | A     | 69  | GLY  | H    | 7.911      | 0.000       | .         |
| 1       | A     | 69  | GLY  | CA   | 45.383     | 0.001       | .         |
| 1       | A     | 69  | GLY  | HA2  | 4.167      | 0.000       | .         |
| 1       | A     | 69  | GLY  | HA3  | 3.963      | 0.000       | .         |
| 1       | A     | 70  | PRO  | CD   | 49.879     | 0.000       | .         |
| 1       | A     | 70  | PRO  | CA   | 63.646     | 0.000       | .         |
| 1       | A     | 70  | PRO  | HA   | 4.405      | 0.000       | .         |
| 1       | A     | 70  | PRO  | CB   | 32.058     | 0.000       | .         |
| 1       | A     | 70  | PRO  | HB2  | 1.885      | 0.000       | .         |
| 1       | A     | 70  | PRO  | HB3  | 2.314      | 0.000       | .         |
| 1       | A     | 70  | PRO  | CG   | 27.12      | 0.000       | .         |
| 1       | A     | 70  | PRO  | HG2  | 2.008      | 0.000       | .         |
| 1       | A     | 70  | PRO  | HG3  | 2.008      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 70  | PRO  | HD2  | 3.626      | 0.000       | .         |
| 1       | A     | 70  | PRO  | HD3  | 3.626      | 0.000       | .         |
| 1       | A     | 71  | ALA  | N    | 121.048    | 0.000       | .         |
| 1       | A     | 71  | ALA  | H    | 7.979      | 0.000       | .         |
| 1       | A     | 71  | ALA  | CA   | 53.004     | 0.002       | .         |
| 1       | A     | 71  | ALA  | HA   | 4.303      | 0.000       | .         |
| 1       | A     | 71  | ALA  | HB1  | 1.394      | 0.002       | .         |
| 1       | A     | 71  | ALA  | HB2  | 1.394      | 0.002       | .         |
| 1       | A     | 71  | ALA  | HB3  | 1.394      | 0.002       | .         |
| 1       | A     | 71  | ALA  | CB   | 19.094     | 0.000       | .         |
| 1       | A     | 71  | ALA  | C    | 177.069    | 0.000       | .         |
| 1       | A     | 72  | LEU  | N    | 118.512    | 0.000       | .         |
| 1       | A     | 72  | LEU  | H    | 7.676      | 0.000       | .         |
| 1       | A     | 72  | LEU  | CA   | 54.13      | 0.005       | .         |
| 1       | A     | 72  | LEU  | HA   | 4.448      | 0.000       | .         |
| 1       | A     | 72  | LEU  | CB   | 44.351     | 0.000       | .         |
| 1       | A     | 72  | LEU  | HB2  | 1.511      | 0.000       | .         |
| 1       | A     | 72  | LEU  | HB3  | 1.555      | 0.000       | .         |
| 1       | A     | 72  | LEU  | CG   | 26.873     | 0.000       | .         |
| 1       | A     | 72  | LEU  | HG   | 1.568      | 0.000       | .         |
| 1       | A     | 72  | LEU  | HD11 | 0.809      | 0.001       | .         |
| 1       | A     | 72  | LEU  | HD12 | 0.809      | 0.001       | .         |
| 1       | A     | 72  | LEU  | HD13 | 0.809      | 0.001       | .         |
| 1       | A     | 72  | LEU  | HD21 | 0.855      | 0.000       | .         |
| 1       | A     | 72  | LEU  | HD22 | 0.855      | 0.000       | .         |
| 1       | A     | 72  | LEU  | HD23 | 0.855      | 0.000       | .         |
| 1       | A     | 72  | LEU  | CD1  | 23.268     | 0.001       | .         |
| 1       | A     | 72  | LEU  | CD2  | 25.451     | 0.002       | .         |
| 1       | A     | 72  | LEU  | C    | 176.665    | 0.000       | .         |
| 1       | A     | 73  | GLY  | N    | 107.479    | 0.000       | .         |
| 1       | A     | 73  | GLY  | H    | 8.453      | 0.000       | .         |
| 1       | A     | 73  | GLY  | CA   | 45.772     | 0.005       | .         |
| 1       | A     | 73  | GLY  | HA2  | 4.015      | 0.000       | .         |
| 1       | A     | 73  | GLY  | HA3  | 4.015      | 0.000       | .         |
| 1       | A     | 74  | GLY  | N    | 108.942    | 0.000       | .         |
| 1       | A     | 74  | GLY  | H    | 8.497      | 0.000       | .         |
| 1       | A     | 74  | GLY  | CA   | 44.341     | 0.000       | .         |
| 1       | A     | 74  | GLY  | HA2  | 3.624      | 0.000       | .         |
| 1       | A     | 74  | GLY  | HA3  | 4.631      | 0.000       | .         |
| 1       | A     | 74  | GLY  | C    | 174.947    | 0.000       | .         |
| 1       | A     | 75  | TRP  | N    | 122.612    | 0.001       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 75  | TRP  | H    | 9.481      | 0.000       | .         |
| 1       | A     | 75  | TRP  | CA   | 57.784     | 0.000       | .         |
| 1       | A     | 75  | TRP  | HA   | 5.19       | 0.000       | .         |
| 1       | A     | 75  | TRP  | CB   | 30.639     | 0.000       | .         |
| 1       | A     | 75  | TRP  | HB2  | 2.967      | 0.000       | .         |
| 1       | A     | 75  | TRP  | HB3  | 3.661      | 0.000       | .         |
| 1       | A     | 75  | TRP  | CD1  | 126.642    | 0.000       | .         |
| 1       | A     | 75  | TRP  | CE3  | 119.583    | 0.001       | .         |
| 1       | A     | 75  | TRP  | NE1  | 127.867    | 0.000       | .         |
| 1       | A     | 75  | TRP  | HD1  | 7.493      | 0.001       | .         |
| 1       | A     | 75  | TRP  | HE3  | 7.209      | 0.001       | .         |
| 1       | A     | 75  | TRP  | CZ2  | 114.468    | 0.001       | .         |
| 1       | A     | 75  | TRP  | HE1  | 9.884      | 0.000       | .         |
| 1       | A     | 75  | TRP  | CH2  | 126.008    | 0.000       | .         |
| 1       | A     | 75  | TRP  | HZ2  | 6.446      | 0.000       | .         |
| 1       | A     | 75  | TRP  | HH2  | 7.044      | 0.000       | .         |
| 1       | A     | 75  | TRP  | C    | 178.743    | 0.000       | .         |
| 1       | A     | 76  | SER  | CA   | 58.797     | 0.000       | .         |
| 1       | A     | 76  | SER  | HA   | 4.925      | 0.000       | .         |
| 1       | A     | 76  | SER  | CB   | 64.837     | 0.000       | .         |
| 1       | A     | 76  | SER  | HB2  | 3.419      | 0.000       | .         |
| 1       | A     | 76  | SER  | HB3  | 4.208      | 0.000       | .         |
| 1       | A     | 77  | SER  | N    | 120.114    | 0.000       | .         |
| 1       | A     | 77  | SER  | H    | 8.461      | 0.000       | .         |
| 1       | A     | 77  | SER  | CA   | 58.798     | 0.000       | .         |
| 1       | A     | 77  | SER  | HA   | 4.935      | 0.000       | .         |
| 1       | A     | 77  | SER  | CB   | 64.913     | 0.000       | .         |
| 1       | A     | 77  | SER  | HB2  | 3.404      | 0.000       | .         |
| 1       | A     | 77  | SER  | HB3  | 3.404      | 0.000       | .         |
| 1       | A     | 77  | SER  | C    | 170.989    | 0.000       | .         |
| 1       | A     | 78  | TYR  | N    | 120.186    | 0.000       | .         |
| 1       | A     | 78  | TYR  | H    | 8.928      | 0.000       | .         |
| 1       | A     | 78  | TYR  | CA   | 56.702     | 0.000       | .         |
| 1       | A     | 78  | TYR  | HA   | 4.664      | 0.000       | .         |
| 1       | A     | 78  | TYR  | CB   | 39.653     | 0.002       | .         |
| 1       | A     | 78  | TYR  | HB2  | 2.556      | 0.005       | .         |
| 1       | A     | 78  | TYR  | HB3  | 2.984      | 0.000       | .         |
| 1       | A     | 78  | TYR  | HD1  | 6.855      | 0.001       | .         |
| 1       | A     | 78  | TYR  | HD2  | 6.855      | 0.001       | .         |
| 1       | A     | 78  | TYR  | HE1  | 6.868      | 0.000       | .         |
| 1       | A     | 78  | TYR  | HE2  | 6.868      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 78  | TYR  | CD1  | 132.326    | 0.000       | .         |
| 1       | A     | 78  | TYR  | CE1  | 118.298    | 0.000       | .         |
| 1       | A     | 78  | TYR  | CE2  | 118.298    | 0.000       | .         |
| 1       | A     | 78  | TYR  | CD2  | 132.326    | 0.000       | .         |
| 1       | A     | 78  | TYR  | C    | 175.037    | 0.000       | .         |
| 1       | A     | 79  | LEU  | N    | 125.78     | 0.000       | .         |
| 1       | A     | 79  | LEU  | H    | 8.904      | 0.000       | .         |
| 1       | A     | 79  | LEU  | CA   | 52.472     | 0.000       | .         |
| 1       | A     | 79  | LEU  | HA   | 4.895      | 0.000       | .         |
| 1       | A     | 79  | LEU  | CB   | 43.296     | 0.001       | .         |
| 1       | A     | 79  | LEU  | HB2  | 0.89       | 0.000       | .         |
| 1       | A     | 79  | LEU  | HB3  | 1.706      | 0.000       | .         |
| 1       | A     | 79  | LEU  | CG   | 27.791     | 0.000       | .         |
| 1       | A     | 79  | LEU  | HG   | 1.265      | 0.000       | .         |
| 1       | A     | 79  | LEU  | HD11 | 0.338      | 0.000       | .         |
| 1       | A     | 79  | LEU  | HD12 | 0.338      | 0.000       | .         |
| 1       | A     | 79  | LEU  | HD13 | 0.338      | 0.000       | .         |
| 1       | A     | 79  | LEU  | HD21 | 0.471      | 0.000       | .         |
| 1       | A     | 79  | LEU  | HD22 | 0.471      | 0.000       | .         |
| 1       | A     | 79  | LEU  | HD23 | 0.471      | 0.000       | .         |
| 1       | A     | 79  | LEU  | CD1  | 21.824     | 0.000       | .         |
| 1       | A     | 79  | LEU  | CD2  | 25.322     | 0.000       | .         |
| 1       | A     | 79  | LEU  | C    | 176.876    | 0.001       | .         |
| 1       | A     | 81  | VAL  | N    | 116.916    | 0.000       | .         |
| 1       | A     | 81  | VAL  | H    | 8.608      | 0.000       | .         |
| 1       | A     | 81  | VAL  | CA   | 59.255     | 0.000       | .         |
| 1       | A     | 81  | VAL  | HA   | 4.862      | 0.000       | .         |
| 1       | A     | 81  | VAL  | CB   | 36.027     | 0.000       | .         |
| 1       | A     | 81  | VAL  | HB   | 2.113      | 0.000       | .         |
| 1       | A     | 81  | VAL  | HG11 | 0.661      | 0.000       | .         |
| 1       | A     | 81  | VAL  | HG12 | 0.661      | 0.000       | .         |
| 1       | A     | 81  | VAL  | HG13 | 0.661      | 0.000       | .         |
| 1       | A     | 81  | VAL  | HG21 | 1.083      | 0.000       | .         |
| 1       | A     | 81  | VAL  | HG22 | 1.083      | 0.000       | .         |
| 1       | A     | 81  | VAL  | HG23 | 1.083      | 0.000       | .         |
| 1       | A     | 81  | VAL  | CG1  | 18.683     | 0.000       | .         |
| 1       | A     | 81  | VAL  | CG2  | 23.869     | 0.000       | .         |
| 1       | A     | 81  | VAL  | C    | 175.037    | 0.000       | .         |
| 1       | A     | 82  | ASP  | N    | 121.088    | 0.000       | .         |
| 1       | A     | 82  | ASP  | H    | 8.836      | 0.000       | .         |
| 1       | A     | 82  | ASP  | CA   | 56.166     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 82  | ASP  | HA   | 4.636      | 0.000       | .         |
| 1       | A     | 82  | ASP  | CB   | 40.809     | 0.000       | .         |
| 1       | A     | 82  | ASP  | HB2  | 2.577      | 0.000       | .         |
| 1       | A     | 82  | ASP  | HB3  | 2.645      | 0.003       | .         |
| 1       | A     | 82  | ASP  | C    | 177.354    | 0.000       | .         |
| 1       | A     | 83  | ASP  | N    | 116.398    | 0.000       | .         |
| 1       | A     | 83  | ASP  | H    | 7.269      | 0.000       | .         |
| 1       | A     | 83  | ASP  | CA   | 53.031     | 0.001       | .         |
| 1       | A     | 83  | ASP  | HA   | 4.495      | 0.000       | .         |
| 1       | A     | 83  | ASP  | CB   | 42.722     | 0.001       | .         |
| 1       | A     | 83  | ASP  | HB2  | 2.397      | 0.000       | .         |
| 1       | A     | 83  | ASP  | HB3  | 2.72       | 0.000       | .         |
| 1       | A     | 83  | ASP  | C    | 176.095    | 0.000       | .         |
| 1       | A     | 84  | ALA  | N    | 129.069    | 0.000       | .         |
| 1       | A     | 84  | ALA  | H    | 9.428      | 0.000       | .         |
| 1       | A     | 84  | ALA  | CA   | 55.492     | 0.000       | .         |
| 1       | A     | 84  | ALA  | HA   | 3.794      | 0.000       | .         |
| 1       | A     | 84  | ALA  | HB1  | 1.113      | 0.000       | .         |
| 1       | A     | 84  | ALA  | HB2  | 1.113      | 0.000       | .         |
| 1       | A     | 84  | ALA  | HB3  | 1.113      | 0.000       | .         |
| 1       | A     | 84  | ALA  | CB   | 17.837     | 0.000       | .         |
| 1       | A     | 84  | ALA  | C    | 177.911    | 0.000       | .         |
| 1       | A     | 86  | ALA  | N    | 125.185    | 0.000       | .         |
| 1       | A     | 86  | ALA  | H    | 8.244      | 0.000       | .         |
| 1       | A     | 86  | ALA  | CA   | 54.341     | 0.000       | .         |
| 1       | A     | 86  | ALA  | HA   | 4.074      | 0.000       | .         |
| 1       | A     | 86  | ALA  | HB1  | 1.363      | 0.000       | .         |
| 1       | A     | 86  | ALA  | HB2  | 1.363      | 0.000       | .         |
| 1       | A     | 86  | ALA  | HB3  | 1.363      | 0.000       | .         |
| 1       | A     | 86  | ALA  | CB   | 17.79      | 0.001       | .         |
| 1       | A     | 86  | ALA  | C    | 181.312    | 0.000       | .         |
| 1       | A     | 88  | ALA  | N    | 118.62     | 0.000       | .         |
| 1       | A     | 88  | ALA  | H    | 8.226      | 0.000       | .         |
| 1       | A     | 88  | ALA  | CA   | 54.988     | 0.000       | .         |
| 1       | A     | 88  | ALA  | HA   | 3.706      | 0.000       | .         |
| 1       | A     | 88  | ALA  | HB1  | 1.516      | 0.000       | .         |
| 1       | A     | 88  | ALA  | HB2  | 1.516      | 0.000       | .         |
| 1       | A     | 88  | ALA  | HB3  | 1.516      | 0.000       | .         |
| 1       | A     | 88  | ALA  | CB   | 18.015     | 0.000       | .         |
| 1       | A     | 88  | ALA  | C    | 179.01     | 0.000       | .         |
| 1       | A     | 91  | VAL  | N    | 115.357    | 0.000       | .         |

*Continued on next page...*



*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 91  | VAL  | H    | 7.819      | 0.000       | .         |
| 1       | A     | 91  | VAL  | CA   | 69.345     | 0.000       | .         |
| 1       | A     | 91  | VAL  | HA   | 3.529      | 0.000       | .         |
| 1       | A     | 91  | VAL  | CB   | 30.295     | 0.003       | .         |
| 1       | A     | 91  | VAL  | HB   | 2.089      | 0.000       | .         |
| 1       | A     | 91  | VAL  | HG11 | 0.795      | 0.000       | .         |
| 1       | A     | 91  | VAL  | HG12 | 0.795      | 0.000       | .         |
| 1       | A     | 91  | VAL  | HG13 | 0.795      | 0.000       | .         |
| 1       | A     | 91  | VAL  | HG21 | 0.927      | 0.000       | .         |
| 1       | A     | 91  | VAL  | HG22 | 0.927      | 0.000       | .         |
| 1       | A     | 91  | VAL  | HG23 | 0.927      | 0.000       | .         |
| 1       | A     | 91  | VAL  | CG1  | 22.189     | 0.000       | .         |
| 1       | A     | 91  | VAL  | CG2  | 24.321     | 0.000       | .         |
| 1       | A     | 91  | VAL  | C    | 175.819    | 0.000       | .         |
| 1       | A     | 92  | PRO  | CD   | 50.422     | 0.000       | .         |
| 1       | A     | 92  | PRO  | CA   | 64.867     | 0.000       | .         |
| 1       | A     | 92  | PRO  | HA   | 4.685      | 0.000       | .         |
| 1       | A     | 92  | PRO  | CB   | 30.951     | 0.000       | .         |
| 1       | A     | 92  | PRO  | HB2  | 1.94       | 0.000       | .         |
| 1       | A     | 92  | PRO  | HB3  | 2.395      | 0.000       | .         |
| 1       | A     | 92  | PRO  | CG   | 28.567     | 0.000       | .         |
| 1       | A     | 92  | PRO  | HG2  | 1.921      | 0.000       | .         |
| 1       | A     | 92  | PRO  | HG3  | 2.154      | 0.000       | .         |
| 1       | A     | 92  | PRO  | HD2  | 3.46       | 0.000       | .         |
| 1       | A     | 92  | PRO  | HD3  | 3.768      | 0.000       | .         |
| 1       | A     | 92  | PRO  | C    | 181.031    | 0.000       | .         |
| 1       | A     | 93  | GLU  | N    | 118.774    | 0.000       | .         |
| 1       | A     | 93  | GLU  | H    | 6.947      | 0.000       | .         |
| 1       | A     | 93  | GLU  | CA   | 58.384     | 0.001       | .         |
| 1       | A     | 93  | GLU  | HA   | 4.139      | 0.000       | .         |
| 1       | A     | 93  | GLU  | CB   | 29.144     | 0.000       | .         |
| 1       | A     | 93  | GLU  | HB2  | 2.166      | 0.000       | .         |
| 1       | A     | 93  | GLU  | HB3  | 2.166      | 0.000       | .         |
| 1       | A     | 93  | GLU  | CG   | 35.909     | 0.000       | .         |
| 1       | A     | 93  | GLU  | HG2  | 2.293      | 0.000       | .         |
| 1       | A     | 93  | GLU  | HG3  | 2.431      | 0.000       | .         |
| 1       | A     | 93  | GLU  | C    | 178.236    | 0.000       | .         |
| 1       | A     | 94  | LEU  | N    | 117.709    | 0.000       | .         |
| 1       | A     | 94  | LEU  | H    | 7.571      | 0.000       | .         |
| 1       | A     | 94  | LEU  | CA   | 54.416     | 0.000       | .         |
| 1       | A     | 94  | LEU  | HA   | 4.405      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 94  | LEU  | CB   | 44.032     | 0.000       | .         |
| 1       | A     | 94  | LEU  | HB2  | 1.767      | 0.000       | .         |
| 1       | A     | 94  | LEU  | HB3  | 1.806      | 0.000       | .         |
| 1       | A     | 94  | LEU  | CG   | 25.737     | 0.001       | .         |
| 1       | A     | 94  | LEU  | HG   | 1.601      | 0.000       | .         |
| 1       | A     | 94  | LEU  | HD11 | 0.801      | 0.000       | .         |
| 1       | A     | 94  | LEU  | HD12 | 0.801      | 0.000       | .         |
| 1       | A     | 94  | LEU  | HD13 | 0.801      | 0.000       | .         |
| 1       | A     | 94  | LEU  | HD21 | 0.362      | 0.000       | .         |
| 1       | A     | 94  | LEU  | HD22 | 0.362      | 0.000       | .         |
| 1       | A     | 94  | LEU  | HD23 | 0.362      | 0.000       | .         |
| 1       | A     | 94  | LEU  | CD1  | 22.627     | 0.000       | .         |
| 1       | A     | 94  | LEU  | CD2  | 25.452     | 0.000       | .         |
| 1       | A     | 94  | LEU  | C    | 176.915    | 0.000       | .         |
| 1       | A     | 95  | GLY  | N    | 105.091    | 0.000       | .         |
| 1       | A     | 95  | GLY  | H    | 7.617      | 0.000       | .         |
| 1       | A     | 95  | GLY  | CA   | 45.247     | 0.000       | .         |
| 1       | A     | 95  | GLY  | HA2  | 3.822      | 0.000       | .         |
| 1       | A     | 95  | GLY  | HA3  | 4.393      | 0.000       | .         |
| 1       | A     | 95  | GLY  | C    | 175.124    | 0.000       | .         |
| 1       | A     | 96  | GLY  | N    | 107.985    | 0.001       | .         |
| 1       | A     | 96  | GLY  | H    | 8.023      | 0.000       | .         |
| 1       | A     | 96  | GLY  | CA   | 43.291     | 0.006       | .         |
| 1       | A     | 96  | GLY  | HA2  | 3.435      | 0.000       | .         |
| 1       | A     | 96  | GLY  | HA3  | 4.044      | 0.000       | .         |
| 1       | A     | 96  | GLY  | C    | 171.448    | 0.000       | .         |
| 1       | A     | 97  | ALA  | N    | 120.487    | 0.000       | .         |
| 1       | A     | 97  | ALA  | H    | 8.488      | 0.000       | .         |
| 1       | A     | 97  | ALA  | CA   | 50.784     | 0.000       | .         |
| 1       | A     | 97  | ALA  | HA   | 4.618      | 0.000       | .         |
| 1       | A     | 97  | ALA  | HB1  | 1.187      | 0.000       | .         |
| 1       | A     | 97  | ALA  | HB2  | 1.187      | 0.000       | .         |
| 1       | A     | 97  | ALA  | HB3  | 1.187      | 0.000       | .         |
| 1       | A     | 97  | ALA  | CB   | 22.369     | 0.000       | .         |
| 1       | A     | 97  | ALA  | C    | 176.403    | 0.000       | .         |
| 1       | A     | 98  | VAL  | N    | 122.906    | 0.000       | .         |
| 1       | A     | 98  | VAL  | H    | 9.189      | 0.000       | .         |
| 1       | A     | 98  | VAL  | CA   | 64.258     | 0.000       | .         |
| 1       | A     | 98  | VAL  | HA   | 3.971      | 0.000       | .         |
| 1       | A     | 98  | VAL  | CB   | 31.575     | 0.001       | .         |
| 1       | A     | 98  | VAL  | HB   | 2.091      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 98  | VAL  | HG11 | 0.891      | 0.000       | .         |
| 1       | A     | 98  | VAL  | HG12 | 0.891      | 0.000       | .         |
| 1       | A     | 98  | VAL  | HG13 | 0.891      | 0.000       | .         |
| 1       | A     | 98  | VAL  | HG21 | 0.995      | 0.000       | .         |
| 1       | A     | 98  | VAL  | HG22 | 0.995      | 0.000       | .         |
| 1       | A     | 98  | VAL  | HG23 | 0.995      | 0.000       | .         |
| 1       | A     | 98  | VAL  | CG1  | 21.759     | 0.001       | .         |
| 1       | A     | 98  | VAL  | CG2  | 22.839     | 0.000       | .         |
| 1       | A     | 98  | VAL  | C    | 175.76     | 0.002       | .         |
| 1       | A     | 99  | LEU  | N    | 128.5      | 0.000       | .         |
| 1       | A     | 99  | LEU  | H    | 9.138      | 0.000       | .         |
| 1       | A     | 99  | LEU  | CA   | 55.559     | 0.000       | .         |
| 1       | A     | 99  | LEU  | HA   | 4.415      | 0.000       | .         |
| 1       | A     | 99  | LEU  | CB   | 42.813     | 0.000       | .         |
| 1       | A     | 99  | LEU  | HB2  | 1.398      | 0.000       | .         |
| 1       | A     | 99  | LEU  | HB3  | 1.398      | 0.000       | .         |
| 1       | A     | 99  | LEU  | CG   | 27.377     | 0.000       | .         |
| 1       | A     | 99  | LEU  | HG   | 1.504      | 0.000       | .         |
| 1       | A     | 99  | LEU  | HD11 | 0.739      | 0.000       | .         |
| 1       | A     | 99  | LEU  | HD12 | 0.739      | 0.000       | .         |
| 1       | A     | 99  | LEU  | HD13 | 0.739      | 0.000       | .         |
| 1       | A     | 99  | LEU  | HD21 | 0.747      | 0.000       | .         |
| 1       | A     | 99  | LEU  | HD22 | 0.747      | 0.000       | .         |
| 1       | A     | 99  | LEU  | HD23 | 0.747      | 0.000       | .         |
| 1       | A     | 99  | LEU  | CD1  | 21.93      | 0.000       | .         |
| 1       | A     | 99  | LEU  | CD2  | 25.183     | 0.000       | .         |
| 1       | A     | 99  | LEU  | C    | 176.934    | 0.000       | .         |
| 1       | A     | 100 | LEU  | N    | 119.087    | 0.000       | .         |
| 1       | A     | 100 | LEU  | H    | 7.729      | 0.000       | .         |
| 1       | A     | 100 | LEU  | CA   | 55.884     | 0.001       | .         |
| 1       | A     | 100 | LEU  | HA   | 4.518      | 0.000       | .         |
| 1       | A     | 100 | LEU  | CB   | 46.089     | 0.001       | .         |
| 1       | A     | 100 | LEU  | HB2  | 1.623      | 0.000       | .         |
| 1       | A     | 100 | LEU  | HB3  | 1.684      | 0.000       | .         |
| 1       | A     | 100 | LEU  | CG   | 27.532     | 0.000       | .         |
| 1       | A     | 100 | LEU  | HG   | 1.59       | 0.000       | .         |
| 1       | A     | 100 | LEU  | HD11 | 0.996      | 0.000       | .         |
| 1       | A     | 100 | LEU  | HD12 | 0.996      | 0.000       | .         |
| 1       | A     | 100 | LEU  | HD13 | 0.996      | 0.000       | .         |
| 1       | A     | 100 | LEU  | HD21 | 1.055      | 0.000       | .         |
| 1       | A     | 100 | LEU  | HD22 | 1.055      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 100 | LEU  | HD23 | 1.055      | 0.000       | .         |
| 1       | A     | 100 | LEU  | CD1  | 26.054     | 0.004       | .         |
| 1       | A     | 100 | LEU  | CD2  | 24.403     | 0.000       | .         |
| 1       | A     | 100 | LEU  | C    | 175.288    | 0.006       | .         |
| 1       | A     | 101 | GLY  | N    | 111.994    | 0.000       | .         |
| 1       | A     | 101 | GLY  | H    | 8.833      | 0.000       | .         |
| 1       | A     | 101 | GLY  | CA   | 44.121     | 0.000       | .         |
| 1       | A     | 101 | GLY  | HA2  | 3.474      | 0.000       | .         |
| 1       | A     | 101 | GLY  | HA3  | 4.567      | 0.000       | .         |
| 1       | A     | 102 | PRO  | CD   | 50.354     | 0.001       | .         |
| 1       | A     | 102 | PRO  | CA   | 61.934     | 0.002       | .         |
| 1       | A     | 102 | PRO  | HA   | 5.223      | 0.000       | .         |
| 1       | A     | 102 | PRO  | CB   | 34.625     | 0.001       | .         |
| 1       | A     | 102 | PRO  | HB2  | 1.876      | 0.000       | .         |
| 1       | A     | 102 | PRO  | HB3  | 1.876      | 0.000       | .         |
| 1       | A     | 102 | PRO  | CG   | 26.225     | 0.000       | .         |
| 1       | A     | 102 | PRO  | HG2  | 1.611      | 0.000       | .         |
| 1       | A     | 102 | PRO  | HG3  | 1.611      | 0.000       | .         |
| 1       | A     | 102 | PRO  | HD2  | 3.462      | 0.000       | .         |
| 1       | A     | 102 | PRO  | HD3  | 3.618      | 0.000       | .         |
| 1       | A     | 102 | PRO  | C    | 175.935    | 0.000       | .         |
| 1       | A     | 103 | ILE  | N    | 121.901    | 0.000       | .         |
| 1       | A     | 103 | ILE  | H    | 9.367      | 0.000       | .         |
| 1       | A     | 103 | ILE  | CA   | 59.492     | 0.000       | .         |
| 1       | A     | 103 | ILE  | HA   | 4.575      | 0.000       | .         |
| 1       | A     | 103 | ILE  | CB   | 42.655     | 0.000       | .         |
| 1       | A     | 103 | ILE  | HB   | 1.78       | 0.000       | .         |
| 1       | A     | 103 | ILE  | HG21 | 0.904      | 0.000       | .         |
| 1       | A     | 103 | ILE  | HG22 | 0.904      | 0.000       | .         |
| 1       | A     | 103 | ILE  | HG23 | 0.904      | 0.000       | .         |
| 1       | A     | 103 | ILE  | CG2  | 17.807     | 0.000       | .         |
| 1       | A     | 103 | ILE  | CG1  | 27.152     | 0.000       | .         |
| 1       | A     | 103 | ILE  | HG12 | 1.44       | 0.000       | .         |
| 1       | A     | 103 | ILE  | HG13 | 1.084      | 0.000       | .         |
| 1       | A     | 103 | ILE  | HD11 | 0.842      | 0.002       | .         |
| 1       | A     | 103 | ILE  | HD12 | 0.842      | 0.002       | .         |
| 1       | A     | 103 | ILE  | HD13 | 0.842      | 0.002       | .         |
| 1       | A     | 103 | ILE  | CD1  | 13.793     | 0.001       | .         |
| 1       | A     | 103 | ILE  | C    | 173.813    | 0.002       | .         |
| 1       | A     | 104 | ASP  | N    | 124.544    | 0.000       | .         |
| 1       | A     | 104 | ASP  | H    | 8.545      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 104 | ASP  | CA   | 54.375     | 0.000       | .         |
| 1       | A     | 104 | ASP  | HA   | 4.83       | 0.000       | .         |
| 1       | A     | 104 | ASP  | CB   | 41.725     | 0.000       | .         |
| 1       | A     | 104 | ASP  | HB2  | 2.497      | 0.000       | .         |
| 1       | A     | 104 | ASP  | HB3  | 2.497      | 0.000       | .         |
| 1       | A     | 104 | ASP  | C    | 175.894    | 0.001       | .         |
| 1       | A     | 105 | ILE  | N    | 123.84     | 0.000       | .         |
| 1       | A     | 105 | ILE  | H    | 8.022      | 0.000       | .         |
| 1       | A     | 105 | ILE  | CA   | 60.233     | 0.001       | .         |
| 1       | A     | 105 | ILE  | HA   | 4.017      | 0.000       | .         |
| 1       | A     | 105 | ILE  | CB   | 36.586     | 0.000       | .         |
| 1       | A     | 105 | ILE  | HB   | 1.36       | 0.000       | .         |
| 1       | A     | 105 | ILE  | HG21 | 0.357      | 0.002       | .         |
| 1       | A     | 105 | ILE  | HG22 | 0.357      | 0.002       | .         |
| 1       | A     | 105 | ILE  | HG23 | 0.357      | 0.002       | .         |
| 1       | A     | 105 | ILE  | CG2  | 16.459     | 0.007       | .         |
| 1       | A     | 105 | ILE  | CG1  | 26.547     | 0.000       | .         |
| 1       | A     | 105 | ILE  | HG12 | 0.829      | 0.000       | .         |
| 1       | A     | 105 | ILE  | HG13 | 0.507      | 0.000       | .         |
| 1       | A     | 105 | ILE  | HD11 | -0.473     | 0.003       | .         |
| 1       | A     | 105 | ILE  | HD12 | -0.473     | 0.003       | .         |
| 1       | A     | 105 | ILE  | HD13 | -0.473     | 0.003       | .         |
| 1       | A     | 105 | ILE  | CD1  | 10.553     | 0.003       | .         |
| 1       | A     | 105 | ILE  | C    | 173.603    | 0.000       | .         |
| 1       | A     | 106 | LEU  | N    | 124.681    | 0.000       | .         |
| 1       | A     | 106 | LEU  | H    | 8.63       | 0.000       | .         |
| 1       | A     | 106 | LEU  | CA   | 56.461     | 0.002       | .         |
| 1       | A     | 106 | LEU  | HA   | 3.827      | 0.000       | .         |
| 1       | A     | 106 | LEU  | CB   | 40.531     | 0.000       | .         |
| 1       | A     | 106 | LEU  | HB2  | 1.605      | 0.000       | .         |
| 1       | A     | 106 | LEU  | HB3  | 1.872      | 0.000       | .         |
| 1       | A     | 106 | LEU  | CG   | 27.171     | 0.000       | .         |
| 1       | A     | 106 | LEU  | HG   | 1.661      | 0.000       | .         |
| 1       | A     | 106 | LEU  | HD11 | 0.92       | 0.000       | .         |
| 1       | A     | 106 | LEU  | HD12 | 0.92       | 0.000       | .         |
| 1       | A     | 106 | LEU  | HD13 | 0.92       | 0.000       | .         |
| 1       | A     | 106 | LEU  | HD21 | 0.985      | 0.000       | .         |
| 1       | A     | 106 | LEU  | HD22 | 0.985      | 0.000       | .         |
| 1       | A     | 106 | LEU  | HD23 | 0.985      | 0.000       | .         |
| 1       | A     | 106 | LEU  | CD1  | 22.951     | 0.000       | .         |
| 1       | A     | 106 | LEU  | CD2  | 25.894     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 107 | ALA  | CA   | 52.704     | 0.000       | .         |
| 1       | A     | 107 | ALA  | HA   | 4.294      | 0.000       | .         |
| 1       | A     | 107 | ALA  | HB1  | 1.369      | 0.000       | .         |
| 1       | A     | 107 | ALA  | HB2  | 1.369      | 0.000       | .         |
| 1       | A     | 107 | ALA  | HB3  | 1.369      | 0.000       | .         |
| 1       | A     | 107 | ALA  | CB   | 19.222     | 0.002       | .         |
| 1       | A     | 108 | GLN  | N    | 118.676    | 0.008       | .         |
| 1       | A     | 108 | GLN  | H    | 8.964      | 0.000       | .         |
| 1       | A     | 108 | GLN  | CA   | 57.066     | 0.000       | .         |
| 1       | A     | 108 | GLN  | HA   | 4.406      | 0.000       | .         |
| 1       | A     | 108 | GLN  | CB   | 30.733     | 0.000       | .         |
| 1       | A     | 108 | GLN  | HB2  | 1.915      | 0.000       | .         |
| 1       | A     | 108 | GLN  | HB3  | 1.915      | 0.000       | .         |
| 1       | A     | 108 | GLN  | CG   | 34.22      | 0.001       | .         |
| 1       | A     | 108 | GLN  | HG2  | 2.326      | 0.000       | .         |
| 1       | A     | 108 | GLN  | HG3  | 2.447      | 0.000       | .         |
| 1       | A     | 108 | GLN  | NE2  | 110.206    | 0.009       | .         |
| 1       | A     | 108 | GLN  | HE21 | 6.656      | 0.008       | .         |
| 1       | A     | 108 | GLN  | HE22 | 7.22       | 0.003       | .         |
| 1       | A     | 109 | GLY  | N    | 104.669    | 0.000       | .         |
| 1       | A     | 109 | GLY  | H    | 7.087      | 0.000       | .         |
| 1       | A     | 109 | GLY  | CA   | 45.046     | 0.002       | .         |
| 1       | A     | 109 | GLY  | HA2  | 2.959      | 0.000       | .         |
| 1       | A     | 109 | GLY  | HA3  | 3.083      | 0.000       | .         |
| 1       | A     | 110 | ARG  | N    | 120.975    | 0.000       | .         |
| 1       | A     | 110 | ARG  | H    | 7.705      | 0.000       | .         |
| 1       | A     | 110 | ARG  | CA   | 54.196     | 0.000       | .         |
| 1       | A     | 110 | ARG  | HA   | 4.827      | 0.000       | .         |
| 1       | A     | 110 | ARG  | CB   | 33.214     | 0.000       | .         |
| 1       | A     | 110 | ARG  | HB2  | 1.74       | 0.000       | .         |
| 1       | A     | 110 | ARG  | HB3  | 1.613      | 0.000       | .         |
| 1       | A     | 110 | ARG  | CG   | 26.905     | 0.000       | .         |
| 1       | A     | 110 | ARG  | HG2  | 1.558      | 0.000       | .         |
| 1       | A     | 110 | ARG  | HG3  | 1.558      | 0.000       | .         |
| 1       | A     | 110 | ARG  | CD   | 43.239     | 0.000       | .         |
| 1       | A     | 110 | ARG  | HD2  | 2.812      | 0.000       | .         |
| 1       | A     | 110 | ARG  | HD3  | 3.098      | 0.000       | .         |
| 1       | A     | 110 | ARG  | NE   | 83.458     | 0.000       | .         |
| 1       | A     | 110 | ARG  | HE   | 7.577      | 0.000       | .         |
| 1       | A     | 110 | ARG  | C    | 172.539    | 0.000       | .         |
| 1       | A     | 111 | MET  | N    | 124.764    | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 111 | MET  | H    | 9.06       | 0.000       | .         |
| 1       | A     | 111 | MET  | CA   | 54.05      | 0.001       | .         |
| 1       | A     | 111 | MET  | HA   | 5.612      | 0.000       | .         |
| 1       | A     | 111 | MET  | CB   | 37.608     | 0.000       | .         |
| 1       | A     | 111 | MET  | HB2  | 1.993      | 0.000       | .         |
| 1       | A     | 111 | MET  | HB3  | 2.159      | 0.000       | .         |
| 1       | A     | 111 | MET  | CG   | 32.43      | 0.001       | .         |
| 1       | A     | 111 | MET  | HG2  | 2.486      | 0.000       | .         |
| 1       | A     | 111 | MET  | HG3  | 2.597      | 0.000       | .         |
| 1       | A     | 111 | MET  | HE1  | 1.754      | 0.005       | .         |
| 1       | A     | 111 | MET  | HE2  | 1.754      | 0.005       | .         |
| 1       | A     | 111 | MET  | HE3  | 1.754      | 0.005       | .         |
| 1       | A     | 111 | MET  | CE   | 17.974     | 0.000       | .         |
| 1       | A     | 111 | MET  | C    | 174.643    | 0.000       | .         |
| 1       | A     | 112 | LEU  | N    | 121.783    | 0.000       | .         |
| 1       | A     | 112 | LEU  | H    | 9.114      | 0.000       | .         |
| 1       | A     | 112 | LEU  | CA   | 55.554     | 0.000       | .         |
| 1       | A     | 112 | LEU  | HA   | 5.044      | 0.000       | .         |
| 1       | A     | 112 | LEU  | CB   | 45.949     | 0.000       | .         |
| 1       | A     | 112 | LEU  | HB2  | 1.622      | 0.000       | .         |
| 1       | A     | 112 | LEU  | HB3  | 1.9        | 0.000       | .         |
| 1       | A     | 112 | LEU  | CG   | 26.421     | 0.000       | .         |
| 1       | A     | 112 | LEU  | HG   | 1.757      | 0.000       | .         |
| 1       | A     | 112 | LEU  | HD11 | 0.87       | 0.000       | .         |
| 1       | A     | 112 | LEU  | HD12 | 0.87       | 0.000       | .         |
| 1       | A     | 112 | LEU  | HD13 | 0.87       | 0.000       | .         |
| 1       | A     | 112 | LEU  | HD21 | 0.965      | 0.000       | .         |
| 1       | A     | 112 | LEU  | HD22 | 0.965      | 0.000       | .         |
| 1       | A     | 112 | LEU  | HD23 | 0.965      | 0.000       | .         |
| 1       | A     | 112 | LEU  | CD1  | 27.013     | 0.000       | .         |
| 1       | A     | 112 | LEU  | CD2  | 27.558     | 0.000       | .         |
| 1       | A     | 112 | LEU  | C    | 174.261    | 0.000       | .         |
| 1       | A     | 113 | LEU  | N    | 121.676    | 0.000       | .         |
| 1       | A     | 113 | LEU  | H    | 8.904      | 0.000       | .         |
| 1       | A     | 113 | LEU  | CA   | 53.975     | 0.001       | .         |
| 1       | A     | 113 | LEU  | HA   | 5.312      | 0.000       | .         |
| 1       | A     | 113 | LEU  | CB   | 46.056     | 0.000       | .         |
| 1       | A     | 113 | LEU  | HB2  | 1.45       | 0.000       | .         |
| 1       | A     | 113 | LEU  | HB3  | 1.702      | 0.000       | .         |
| 1       | A     | 113 | LEU  | CG   | 27.359     | 0.000       | .         |
| 1       | A     | 113 | LEU  | HG   | 1.847      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 113 | LEU  | HD11 | 0.964      | 0.001       | .         |
| 1       | A     | 113 | LEU  | HD12 | 0.964      | 0.001       | .         |
| 1       | A     | 113 | LEU  | HD13 | 0.964      | 0.001       | .         |
| 1       | A     | 113 | LEU  | HD21 | 1.006      | 0.005       | .         |
| 1       | A     | 113 | LEU  | HD22 | 1.006      | 0.005       | .         |
| 1       | A     | 113 | LEU  | HD23 | 1.006      | 0.005       | .         |
| 1       | A     | 113 | LEU  | CD1  | 24.138     | 0.000       | .         |
| 1       | A     | 113 | LEU  | CD2  | 25.334     | 0.000       | .         |
| 1       | A     | 113 | LEU  | C    | 175.18     | 0.000       | .         |
| 1       | A     | 114 | ALA  | N    | 127.385    | 0.000       | .         |
| 1       | A     | 114 | ALA  | H    | 9.738      | 0.000       | .         |
| 1       | A     | 114 | ALA  | CA   | 49.837     | 0.000       | .         |
| 1       | A     | 114 | ALA  | HA   | 5.376      | 0.000       | .         |
| 1       | A     | 114 | ALA  | HB1  | 1.367      | 0.000       | .         |
| 1       | A     | 114 | ALA  | HB2  | 1.367      | 0.000       | .         |
| 1       | A     | 114 | ALA  | HB3  | 1.367      | 0.000       | .         |
| 1       | A     | 114 | ALA  | CB   | 22.961     | 0.000       | .         |
| 1       | A     | 114 | ALA  | C    | 174.191    | 0.000       | .         |
| 1       | A     | 115 | GLY  | N    | 107.004    | 0.000       | .         |
| 1       | A     | 115 | GLY  | H    | 9.436      | 0.000       | .         |
| 1       | A     | 115 | GLY  | CA   | 43.264     | 0.000       | .         |
| 1       | A     | 115 | GLY  | HA2  | 3.319      | 0.000       | .         |
| 1       | A     | 115 | GLY  | HA3  | 5.095      | 0.001       | .         |
| 1       | A     | 115 | GLY  | C    | 173.094    | 0.000       | .         |
| 1       | A     | 116 | ASP  | N    | 122.539    | 0.001       | .         |
| 1       | A     | 116 | ASP  | H    | 8.051      | 0.000       | .         |
| 1       | A     | 116 | ASP  | CA   | 51.67      | 0.000       | .         |
| 1       | A     | 116 | ASP  | HA   | 3.17       | 0.000       | .         |
| 1       | A     | 116 | ASP  | CB   | 39.263     | 0.002       | .         |
| 1       | A     | 116 | ASP  | HB2  | 2.472      | 0.000       | .         |
| 1       | A     | 116 | ASP  | HB3  | 2.633      | 0.000       | .         |
| 1       | A     | 116 | ASP  | C    | 175.339    | 0.000       | .         |
| 1       | A     | 117 | PRO  | CD   | 50.391     | 0.000       | .         |
| 1       | A     | 117 | PRO  | CA   | 65.75      | 0.001       | .         |
| 1       | A     | 117 | PRO  | HA   | 4.127      | 0.000       | .         |
| 1       | A     | 117 | PRO  | CB   | 31.598     | 0.000       | .         |
| 1       | A     | 117 | PRO  | HB2  | 2.393      | 0.000       | .         |
| 1       | A     | 117 | PRO  | HB3  | 2.393      | 0.000       | .         |
| 1       | A     | 117 | PRO  | CG   | 28.429     | 0.000       | .         |
| 1       | A     | 117 | PRO  | HG2  | 1.498      | 0.000       | .         |
| 1       | A     | 117 | PRO  | HG3  | 1.498      | 0.000       | .         |

*Continued on next page...*



*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 117 | PRO  | HD2  | 3.114      | 0.000       | .         |
| 1       | A     | 117 | PRO  | HD3  | 2.17       | 0.000       | .         |
| 1       | A     | 117 | PRO  | C    | 177.796    | 0.000       | .         |
| 1       | A     | 118 | SER  | N    | 111.97     | 0.000       | .         |
| 1       | A     | 118 | SER  | H    | 7.469      | 0.000       | .         |
| 1       | A     | 118 | SER  | CA   | 58.902     | 0.000       | .         |
| 1       | A     | 118 | SER  | HA   | 4.308      | 0.000       | .         |
| 1       | A     | 118 | SER  | CB   | 62.924     | 0.000       | .         |
| 1       | A     | 118 | SER  | HB2  | 3.455      | 0.000       | .         |
| 1       | A     | 118 | SER  | HB3  | 3.664      | 0.000       | .         |
| 1       | A     | 118 | SER  | C    | 173.708    | 0.005       | .         |
| 1       | A     | 119 | GLY  | N    | 109.116    | 0.000       | .         |
| 1       | A     | 119 | GLY  | H    | 8.295      | 0.000       | .         |
| 1       | A     | 119 | GLY  | CA   | 44.71      | 0.002       | .         |
| 1       | A     | 119 | GLY  | HA2  | 3.426      | 0.008       | .         |
| 1       | A     | 119 | GLY  | HA3  | 4.05       | 0.000       | .         |
| 1       | A     | 119 | GLY  | C    | 175.185    | 0.000       | .         |
| 1       | A     | 120 | HIS  | N    | 120.766    | 0.000       | .         |
| 1       | A     | 120 | HIS  | H    | 8.155      | 0.000       | .         |
| 1       | A     | 120 | HIS  | CA   | 55.657     | 0.000       | .         |
| 1       | A     | 120 | HIS  | HA   | 4.792      | 0.000       | .         |
| 1       | A     | 120 | HIS  | CB   | 27.043     | 0.000       | .         |
| 1       | A     | 120 | HIS  | HB2  | 3.421      | 0.000       | .         |
| 1       | A     | 120 | HIS  | HB3  | 3.617      | 0.000       | .         |
| 1       | A     | 120 | HIS  | CD2  | 120.461    | 0.000       | .         |
| 1       | A     | 120 | HIS  | HD2  | 7.396      | 0.000       | .         |
| 1       | A     | 120 | HIS  | C    | 174.599    | 0.002       | .         |
| 1       | A     | 121 | ARG  | N    | 124.265    | 0.000       | .         |
| 1       | A     | 121 | ARG  | H    | 8.577      | 0.000       | .         |
| 1       | A     | 121 | ARG  | CA   | 56.012     | 0.001       | .         |
| 1       | A     | 121 | ARG  | HA   | 5.114      | 0.000       | .         |
| 1       | A     | 121 | ARG  | CB   | 31.887     | 0.000       | .         |
| 1       | A     | 121 | ARG  | HB2  | 1.871      | 0.000       | .         |
| 1       | A     | 121 | ARG  | HB3  | 1.994      | 0.000       | .         |
| 1       | A     | 121 | ARG  | CG   | 27.272     | 0.000       | .         |
| 1       | A     | 121 | ARG  | HG2  | 1.517      | 0.000       | .         |
| 1       | A     | 121 | ARG  | HG3  | 1.698      | 0.000       | .         |
| 1       | A     | 121 | ARG  | CD   | 43.925     | 0.000       | .         |
| 1       | A     | 121 | ARG  | HD2  | 3.226      | 0.000       | .         |
| 1       | A     | 121 | ARG  | HD3  | 3.38       | 0.000       | .         |
| 1       | A     | 121 | ARG  | NE   | 84.359     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 121 | ARG  | HE   | 7.18       | 0.000       | .         |
| 1       | A     | 121 | ARG  | C    | 176.311    | 0.000       | .         |
| 1       | A     | 122 | VAL  | N    | 128.718    | 0.000       | .         |
| 1       | A     | 122 | VAL  | H    | 10.054     | 0.000       | .         |
| 1       | A     | 122 | VAL  | CA   | 60.966     | 0.000       | .         |
| 1       | A     | 122 | VAL  | HA   | 4.231      | 0.000       | .         |
| 1       | A     | 122 | VAL  | CB   | 35.842     | 0.000       | .         |
| 1       | A     | 122 | VAL  | HB   | 2.2        | 0.000       | .         |
| 1       | A     | 122 | VAL  | HG11 | 1.106      | 0.000       | .         |
| 1       | A     | 122 | VAL  | HG12 | 1.106      | 0.000       | .         |
| 1       | A     | 122 | VAL  | HG13 | 1.106      | 0.000       | .         |
| 1       | A     | 122 | VAL  | HG21 | 0.552      | 0.000       | .         |
| 1       | A     | 122 | VAL  | HG22 | 0.552      | 0.000       | .         |
| 1       | A     | 122 | VAL  | HG23 | 0.552      | 0.000       | .         |
| 1       | A     | 122 | VAL  | CG1  | 17.732     | 0.003       | .         |
| 1       | A     | 122 | VAL  | CG2  | 20.96      | 0.000       | .         |
| 1       | A     | 123 | GLY  | N    | 115.491    | 0.000       | .         |
| 1       | A     | 123 | GLY  | H    | 8.436      | 0.000       | .         |
| 1       | A     | 123 | GLY  | CA   | 44.853     | 0.000       | .         |
| 1       | A     | 123 | GLY  | HA2  | 3.06       | 0.000       | .         |
| 1       | A     | 123 | GLY  | HA3  | 4.987      | 0.000       | .         |
| 1       | A     | 123 | GLY  | C    | 172.619    | 0.000       | .         |
| 1       | A     | 124 | LEU  | N    | 124.02     | 0.000       | .         |
| 1       | A     | 124 | LEU  | H    | 9.463      | 0.000       | .         |
| 1       | A     | 124 | LEU  | CA   | 53.506     | 0.001       | .         |
| 1       | A     | 124 | LEU  | HA   | 5.906      | 0.000       | .         |
| 1       | A     | 124 | LEU  | CB   | 43.339     | 0.000       | .         |
| 1       | A     | 124 | LEU  | HB2  | 1.451      | 0.000       | .         |
| 1       | A     | 124 | LEU  | HB3  | 1.878      | 0.000       | .         |
| 1       | A     | 124 | LEU  | CG   | 27.393     | 0.000       | .         |
| 1       | A     | 124 | LEU  | HG   | 1.712      | 0.000       | .         |
| 1       | A     | 124 | LEU  | HD11 | 1.074      | 0.000       | .         |
| 1       | A     | 124 | LEU  | HD12 | 1.074      | 0.000       | .         |
| 1       | A     | 124 | LEU  | HD13 | 1.074      | 0.000       | .         |
| 1       | A     | 124 | LEU  | HD21 | 0.795      | 0.000       | .         |
| 1       | A     | 124 | LEU  | HD22 | 0.795      | 0.000       | .         |
| 1       | A     | 124 | LEU  | HD23 | 0.795      | 0.000       | .         |
| 1       | A     | 124 | LEU  | CD1  | 24.634     | 0.000       | .         |
| 1       | A     | 124 | LEU  | CD2  | 25.83      | 0.000       | .         |
| 1       | A     | 124 | LEU  | C    | 175.119    | 0.001       | .         |
| 1       | A     | 125 | TRP  | N    | 123.117    | 0.001       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 125 | TRP  | H    | 8.951      | 0.000       | .         |
| 1       | A     | 125 | TRP  | CA   | 54.988     | 0.000       | .         |
| 1       | A     | 125 | TRP  | HA   | 5.442      | 0.000       | .         |
| 1       | A     | 125 | TRP  | CB   | 33.97      | 0.000       | .         |
| 1       | A     | 125 | TRP  | HB2  | 2.953      | 0.005       | .         |
| 1       | A     | 125 | TRP  | HB3  | 3.16       | 0.000       | .         |
| 1       | A     | 125 | TRP  | CD1  | 126.321    | 0.000       | .         |
| 1       | A     | 125 | TRP  | NE1  | 126.843    | 0.001       | .         |
| 1       | A     | 125 | TRP  | HD1  | 7.001      | 0.000       | .         |
| 1       | A     | 125 | TRP  | CZ2  | 113.163    | 0.000       | .         |
| 1       | A     | 125 | TRP  | HE1  | 9.141      | 0.000       | .         |
| 1       | A     | 125 | TRP  | CH2  | 121.943    | 0.001       | .         |
| 1       | A     | 125 | TRP  | HZ2  | 6.515      | 0.000       | .         |
| 1       | A     | 125 | TRP  | HH2  | 5.745      | 0.000       | .         |
| 1       | A     | 125 | TRP  | C    | 174.13     | 0.001       | .         |
| 1       | A     | 126 | GLN  | N    | 130.329    | 0.000       | .         |
| 1       | A     | 126 | GLN  | H    | 8.935      | 0.000       | .         |
| 1       | A     | 126 | GLN  | CA   | 52.527     | 0.001       | .         |
| 1       | A     | 126 | GLN  | HA   | 4.942      | 0.000       | .         |
| 1       | A     | 126 | GLN  | CB   | 29.882     | 0.000       | .         |
| 1       | A     | 126 | GLN  | HB2  | 1.738      | 0.000       | .         |
| 1       | A     | 126 | GLN  | HB3  | 1.738      | 0.000       | .         |
| 1       | A     | 126 | GLN  | CG   | 32.328     | 0.000       | .         |
| 1       | A     | 126 | GLN  | HG2  | 2.3        | 0.000       | .         |
| 1       | A     | 126 | GLN  | HG3  | 2.3        | 0.000       | .         |
| 1       | A     | 126 | GLN  | NE2  | 112.115    | 0.005       | .         |
| 1       | A     | 126 | GLN  | HE21 | 7.091      | 0.000       | .         |
| 1       | A     | 126 | GLN  | HE22 | 7.61       | 0.000       | .         |
| 1       | A     | 126 | GLN  | C    | 173.921    | 0.000       | .         |
| 1       | A     | 127 | ALA  | N    | 130.025    | 0.000       | .         |
| 1       | A     | 127 | ALA  | H    | 8.684      | 0.000       | .         |
| 1       | A     | 127 | ALA  | CA   | 54.019     | 0.001       | .         |
| 1       | A     | 127 | ALA  | HA   | 3.776      | 0.000       | .         |
| 1       | A     | 127 | ALA  | HB1  | 1.475      | 0.000       | .         |
| 1       | A     | 127 | ALA  | HB2  | 1.475      | 0.000       | .         |
| 1       | A     | 127 | ALA  | HB3  | 1.475      | 0.000       | .         |
| 1       | A     | 127 | ALA  | CB   | 20.127     | 0.000       | .         |
| 1       | A     | 127 | ALA  | C    | 178.23     | 0.002       | .         |
| 1       | A     | 128 | LYS  | N    | 124.63     | 0.000       | .         |
| 1       | A     | 128 | LYS  | H    | 7.917      | 0.000       | .         |
| 1       | A     | 128 | LYS  | CA   | 57.384     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 128 | LYS  | HA   | 4.394      | 0.000       | .         |
| 1       | A     | 128 | LYS  | CB   | 31.67      | 0.000       | .         |
| 1       | A     | 128 | LYS  | HB2  | 1.161      | 0.000       | .         |
| 1       | A     | 128 | LYS  | HB3  | 1.737      | 0.000       | .         |
| 1       | A     | 128 | LYS  | CG   | 25.297     | 0.001       | .         |
| 1       | A     | 128 | LYS  | HG2  | 1.027      | 0.000       | .         |
| 1       | A     | 128 | LYS  | HG3  | 1.285      | 0.000       | .         |
| 1       | A     | 128 | LYS  | CD   | 29.067     | 0.002       | .         |
| 1       | A     | 128 | LYS  | HD2  | 1.342      | 0.000       | .         |
| 1       | A     | 128 | LYS  | HD3  | 1.436      | 0.000       | .         |
| 1       | A     | 128 | LYS  | CE   | 41.937     | 0.000       | .         |
| 1       | A     | 128 | LYS  | HE2  | 2.571      | 0.000       | .         |
| 1       | A     | 128 | LYS  | HE3  | 2.731      | 0.000       | .         |
| 1       | A     | 128 | LYS  | C    | 175.219    | 0.000       | .         |
| 1       | A     | 129 | GLU  | N    | 117.681    | 0.000       | .         |
| 1       | A     | 129 | GLU  | H    | 8.038      | 0.000       | .         |
| 1       | A     | 129 | GLU  | CA   | 58.287     | 0.000       | .         |
| 1       | A     | 129 | GLU  | HA   | 4.245      | 0.000       | .         |
| 1       | A     | 129 | GLU  | CB   | 30.322     | 0.000       | .         |
| 1       | A     | 129 | GLU  | HB2  | 1.95       | 0.000       | .         |
| 1       | A     | 129 | GLU  | HB3  | 2.158      | 0.000       | .         |
| 1       | A     | 129 | GLU  | CG   | 36.964     | 0.002       | .         |
| 1       | A     | 129 | GLU  | HG2  | 2.265      | 0.000       | .         |
| 1       | A     | 129 | GLU  | HG3  | 2.51       | 0.000       | .         |
| 1       | A     | 129 | GLU  | C    | 176.084    | 0.000       | .         |
| 1       | A     | 130 | HIS  | N    | 122.206    | 0.000       | .         |
| 1       | A     | 130 | HIS  | H    | 9.053      | 0.000       | .         |
| 1       | A     | 130 | HIS  | CA   | 58.02      | 0.000       | .         |
| 1       | A     | 130 | HIS  | HA   | 4.89       | 0.000       | .         |
| 1       | A     | 130 | HIS  | CB   | 33.531     | 0.000       | .         |
| 1       | A     | 130 | HIS  | HB2  | 3.138      | 0.000       | .         |
| 1       | A     | 130 | HIS  | HB3  | 3.208      | 0.000       | .         |
| 1       | A     | 130 | HIS  | C    | 175.619    | 0.000       | .         |
| 1       | A     | 131 | THR  | N    | 113.61     | 0.000       | .         |
| 1       | A     | 131 | THR  | H    | 8.123      | 0.000       | .         |
| 1       | A     | 131 | THR  | CA   | 61.485     | 0.001       | .         |
| 1       | A     | 131 | THR  | HA   | 4.43       | 0.000       | .         |
| 1       | A     | 131 | THR  | CB   | 68.666     | 0.000       | .         |
| 1       | A     | 131 | THR  | HB   | 4.609      | 0.000       | .         |
| 1       | A     | 131 | THR  | HG21 | 1.102      | 0.000       | .         |
| 1       | A     | 131 | THR  | HG22 | 1.102      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 131 | THR  | HG23 | 1.102      | 0.000       | .         |
| 1       | A     | 131 | THR  | CG2  | 21.633     | 0.000       | .         |
| 1       | A     | 131 | THR  | C    | 174.424    | 0.000       | .         |
| 1       | A     | 132 | GLY  | N    | 108.736    | 0.000       | .         |
| 1       | A     | 132 | GLY  | H    | 7.569      | 0.000       | .         |
| 1       | A     | 132 | GLY  | CA   | 45.322     | 0.000       | .         |
| 1       | A     | 132 | GLY  | HA2  | 3.92       | 0.000       | .         |
| 1       | A     | 132 | GLY  | HA3  | 4.927      | 0.000       | .         |
| 1       | A     | 132 | GLY  | C    | 174.071    | 0.000       | .         |
| 1       | A     | 133 | SER  | N    | 116.53     | 0.000       | .         |
| 1       | A     | 133 | SER  | H    | 8.93       | 0.000       | .         |
| 1       | A     | 133 | SER  | CA   | 60.143     | 0.000       | .         |
| 1       | A     | 133 | SER  | HA   | 4.565      | 0.000       | .         |
| 1       | A     | 133 | SER  | CB   | 64.226     | 0.001       | .         |
| 1       | A     | 133 | SER  | HB2  | 3.925      | 0.000       | .         |
| 1       | A     | 133 | SER  | HB3  | 4.113      | 0.000       | .         |
| 1       | A     | 133 | SER  | C    | 176.838    | 0.000       | .         |
| 1       | A     | 134 | GLY  | N    | 113.363    | 0.000       | .         |
| 1       | A     | 134 | GLY  | H    | 8.939      | 0.000       | .         |
| 1       | A     | 134 | GLY  | CA   | 45.326     | 0.000       | .         |
| 1       | A     | 134 | GLY  | HA2  | 3.845      | 0.000       | .         |
| 1       | A     | 134 | GLY  | HA3  | 4.381      | 0.000       | .         |
| 1       | A     | 135 | PRO  | CD   | 49.565     | 0.000       | .         |
| 1       | A     | 135 | PRO  | CA   | 63.277     | 0.001       | .         |
| 1       | A     | 135 | PRO  | HA   | 4.333      | 0.000       | .         |
| 1       | A     | 135 | PRO  | CB   | 32.039     | 0.000       | .         |
| 1       | A     | 135 | PRO  | HB2  | 1.777      | 0.000       | .         |
| 1       | A     | 135 | PRO  | HB3  | 2.27       | 0.000       | .         |
| 1       | A     | 135 | PRO  | CG   | 27.116     | 0.000       | .         |
| 1       | A     | 135 | PRO  | HG2  | 1.995      | 0.000       | .         |
| 1       | A     | 135 | PRO  | HG3  | 1.995      | 0.000       | .         |
| 1       | A     | 135 | PRO  | HD2  | 3.669      | 0.000       | .         |
| 1       | A     | 135 | PRO  | HD3  | 3.669      | 0.000       | .         |
| 1       | A     | 136 | ASP  | N    | 121.766    | 0.000       | .         |
| 1       | A     | 136 | ASP  | H    | 8.537      | 0.000       | .         |
| 1       | A     | 136 | ASP  | CA   | 53.927     | 0.005       | .         |
| 1       | A     | 136 | ASP  | HA   | 4.323      | 0.001       | .         |
| 1       | A     | 136 | ASP  | CB   | 39.842     | 0.002       | .         |
| 1       | A     | 136 | ASP  | HB2  | 2.625      | 0.000       | .         |
| 1       | A     | 136 | ASP  | HB3  | 2.777      | 0.000       | .         |
| 1       | A     | 136 | ASP  | C    | 176.298    | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 137 | ASP  | N    | 125.584    | 0.000       | .         |
| 1       | A     | 137 | ASP  | H    | 8.18       | 0.000       | .         |
| 1       | A     | 137 | ASP  | CA   | 52.789     | 0.005       | .         |
| 1       | A     | 137 | ASP  | HA   | 4.63       | 0.000       | .         |
| 1       | A     | 137 | ASP  | CB   | 41.229     | 0.001       | .         |
| 1       | A     | 137 | ASP  | HB2  | 2.334      | 0.001       | .         |
| 1       | A     | 137 | ASP  | HB3  | 2.891      | 0.000       | .         |
| 1       | A     | 137 | ASP  | C    | 176.128    | 0.001       | .         |
| 1       | A     | 138 | GLY  | N    | 107.164    | 0.000       | .         |
| 1       | A     | 138 | GLY  | H    | 7.732      | 0.000       | .         |
| 1       | A     | 138 | GLY  | CA   | 44.28      | 0.001       | .         |
| 1       | A     | 138 | GLY  | HA2  | 3.688      | 0.001       | .         |
| 1       | A     | 138 | GLY  | HA3  | 4.325      | 0.001       | .         |
| 1       | A     | 138 | GLY  | C    | 172.669    | 0.000       | .         |
| 1       | A     | 139 | ILE  | N    | 117.904    | 0.000       | .         |
| 1       | A     | 139 | ILE  | H    | 8.319      | 0.000       | .         |
| 1       | A     | 139 | ILE  | CA   | 62.849     | 0.000       | .         |
| 1       | A     | 139 | ILE  | HA   | 3.408      | 0.004       | .         |
| 1       | A     | 139 | ILE  | CB   | 37.482     | 0.000       | .         |
| 1       | A     | 139 | ILE  | HB   | 1.862      | 0.000       | .         |
| 1       | A     | 139 | ILE  | HG21 | 1.062      | 0.001       | .         |
| 1       | A     | 139 | ILE  | HG22 | 1.062      | 0.001       | .         |
| 1       | A     | 139 | ILE  | HG23 | 1.062      | 0.001       | .         |
| 1       | A     | 139 | ILE  | CG2  | 18.229     | 0.000       | .         |
| 1       | A     | 139 | ILE  | CG1  | 27.46      | 0.000       | .         |
| 1       | A     | 139 | ILE  | HG12 | 1.219      | 0.000       | .         |
| 1       | A     | 139 | ILE  | HG13 | 1.576      | 0.000       | .         |
| 1       | A     | 139 | ILE  | HD11 | 0.816      | 0.000       | .         |
| 1       | A     | 139 | ILE  | HD12 | 0.816      | 0.000       | .         |
| 1       | A     | 139 | ILE  | HD13 | 0.816      | 0.000       | .         |
| 1       | A     | 139 | ILE  | CD1  | 12.733     | 0.000       | .         |
| 1       | A     | 139 | ILE  | C    | 177.906    | 0.000       | .         |
| 1       | A     | 140 | GLY  | N    | 116.622    | 0.000       | .         |
| 1       | A     | 140 | GLY  | H    | 9.652      | 0.000       | .         |
| 1       | A     | 140 | GLY  | CA   | 45.083     | 0.004       | .         |
| 1       | A     | 140 | GLY  | HA2  | 3.227      | 0.001       | .         |
| 1       | A     | 140 | GLY  | HA3  | 4.381      | 0.000       | .         |
| 1       | A     | 140 | GLY  | C    | 171.946    | 0.000       | .         |
| 1       | A     | 141 | ALA  | N    | 118.824    | 0.001       | .         |
| 1       | A     | 141 | ALA  | H    | 7.543      | 0.000       | .         |
| 1       | A     | 141 | ALA  | CA   | 51.235     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 141 | ALA  | HA   | 4.344      | 0.000       | .         |
| 1       | A     | 141 | ALA  | HB1  | 1.559      | 0.000       | .         |
| 1       | A     | 141 | ALA  | HB2  | 1.559      | 0.000       | .         |
| 1       | A     | 141 | ALA  | HB3  | 1.559      | 0.000       | .         |
| 1       | A     | 141 | ALA  | CB   | 19.958     | 0.000       | .         |
| 1       | A     | 141 | ALA  | C    | 176.261    | 0.001       | .         |
| 1       | A     | 142 | TYR  | N    | 119.136    | 0.000       | .         |
| 1       | A     | 142 | TYR  | H    | 8.694      | 0.000       | .         |
| 1       | A     | 142 | TYR  | CA   | 56.285     | 0.000       | .         |
| 1       | A     | 142 | TYR  | HA   | 4.549      | 0.000       | .         |
| 1       | A     | 142 | TYR  | CB   | 38.207     | 0.003       | .         |
| 1       | A     | 142 | TYR  | HB2  | 2.868      | 0.000       | .         |
| 1       | A     | 142 | TYR  | HB3  | 2.582      | 0.000       | .         |
| 1       | A     | 142 | TYR  | HD1  | 6.311      | 0.000       | .         |
| 1       | A     | 142 | TYR  | HD2  | 6.311      | 0.000       | .         |
| 1       | A     | 142 | TYR  | HE1  | 7.053      | 0.000       | .         |
| 1       | A     | 142 | TYR  | HE2  | 7.053      | 0.000       | .         |
| 1       | A     | 142 | TYR  | CD1  | 130.631    | 0.000       | .         |
| 1       | A     | 142 | TYR  | CE1  | 118.169    | 0.000       | .         |
| 1       | A     | 142 | TYR  | CE2  | 118.169    | 0.000       | .         |
| 1       | A     | 142 | TYR  | CD2  | 130.631    | 0.000       | .         |
| 1       | A     | 142 | TYR  | C    | 175.106    | 0.000       | .         |
| 1       | A     | 143 | THR  | N    | 127.833    | 0.000       | .         |
| 1       | A     | 143 | THR  | H    | 8.534      | 0.000       | .         |
| 1       | A     | 143 | THR  | CA   | 65.489     | 0.000       | .         |
| 1       | A     | 143 | THR  | HA   | 4.195      | 0.000       | .         |
| 1       | A     | 143 | THR  | CB   | 69.488     | 0.001       | .         |
| 1       | A     | 143 | THR  | HB   | 3.363      | 0.000       | .         |
| 1       | A     | 143 | THR  | HG21 | 0.98       | 0.000       | .         |
| 1       | A     | 143 | THR  | HG22 | 0.98       | 0.000       | .         |
| 1       | A     | 143 | THR  | HG23 | 0.98       | 0.000       | .         |
| 1       | A     | 143 | THR  | CG2  | 22.471     | 0.002       | .         |
| 1       | A     | 143 | THR  | C    | 174.2      | 0.000       | .         |
| 1       | A     | 144 | ARG  | N    | 109.282    | 0.000       | .         |
| 1       | A     | 144 | ARG  | H    | 6.832      | 0.000       | .         |
| 1       | A     | 144 | ARG  | CA   | 55.32      | 0.000       | .         |
| 1       | A     | 144 | ARG  | HA   | 3.644      | 0.000       | .         |
| 1       | A     | 144 | ARG  | CB   | 30.234     | 0.000       | .         |
| 1       | A     | 144 | ARG  | C    | 173.593    | 0.000       | .         |
| 1       | A     | 145 | SER  | N    | 110.089    | 0.000       | .         |
| 1       | A     | 145 | SER  | H    | 6.303      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 145 | SER  | CA   | 58.23      | 0.001       | .         |
| 1       | A     | 145 | SER  | HA   | 5.798      | 0.001       | .         |
| 1       | A     | 145 | SER  | CB   | 66.655     | 0.000       | .         |
| 1       | A     | 145 | SER  | HB2  | 3.462      | 0.002       | .         |
| 1       | A     | 145 | SER  | HB3  | 4.197      | 0.000       | .         |
| 1       | A     | 145 | SER  | C    | 171.576    | 0.000       | .         |
| 1       | A     | 146 | GLU  | N    | 119.046    | 0.000       | .         |
| 1       | A     | 146 | GLU  | H    | 8.525      | 0.000       | .         |
| 1       | A     | 146 | GLU  | CA   | 55.092     | 0.000       | .         |
| 1       | A     | 146 | GLU  | HA   | 5.059      | 0.007       | .         |
| 1       | A     | 146 | GLU  | CB   | 33.335     | 0.000       | .         |
| 1       | A     | 146 | GLU  | HB2  | 1.7        | 0.000       | .         |
| 1       | A     | 146 | GLU  | HB3  | 1.7        | 0.000       | .         |
| 1       | A     | 146 | GLU  | CG   | 37.66      | 0.001       | .         |
| 1       | A     | 146 | GLU  | HG2  | 2.683      | 0.000       | .         |
| 1       | A     | 146 | GLU  | HG3  | 2.683      | 0.000       | .         |
| 1       | A     | 146 | GLU  | C    | 173.09     | 0.005       | .         |
| 1       | A     | 147 | LEU  | N    | 124.825    | 0.000       | .         |
| 1       | A     | 147 | LEU  | H    | 7.983      | 0.000       | .         |
| 1       | A     | 147 | LEU  | CA   | 52.423     | 0.000       | .         |
| 1       | A     | 147 | LEU  | HA   | 3.602      | 0.000       | .         |
| 1       | A     | 147 | LEU  | CB   | 40.321     | 0.002       | .         |
| 1       | A     | 147 | LEU  | HB2  | -1.791     | 0.000       | .         |
| 1       | A     | 147 | LEU  | HB3  | -1.791     | 0.000       | .         |
| 1       | A     | 147 | LEU  | CG   | 26.282     | 0.000       | .         |
| 1       | A     | 147 | LEU  | HG   | 0.519      | 0.000       | .         |
| 1       | A     | 147 | LEU  | HD11 | -0.554     | 0.000       | .         |
| 1       | A     | 147 | LEU  | HD12 | -0.554     | 0.000       | .         |
| 1       | A     | 147 | LEU  | HD13 | -0.554     | 0.000       | .         |
| 1       | A     | 147 | LEU  | HD21 | 0.598      | 0.000       | .         |
| 1       | A     | 147 | LEU  | HD22 | 0.598      | 0.000       | .         |
| 1       | A     | 147 | LEU  | HD23 | 0.598      | 0.000       | .         |
| 1       | A     | 147 | LEU  | CD1  | 19.992     | 0.000       | .         |
| 1       | A     | 147 | LEU  | CD2  | 26.07      | 0.000       | .         |
| 1       | A     | 147 | LEU  | C    | 173.274    | 0.002       | .         |
| 1       | A     | 148 | LEU  | N    | 130.321    | 0.000       | .         |
| 1       | A     | 148 | LEU  | H    | 8.352      | 0.000       | .         |
| 1       | A     | 148 | LEU  | CA   | 53.631     | 0.000       | .         |
| 1       | A     | 148 | LEU  | HA   | 4.721      | 0.000       | .         |
| 1       | A     | 148 | LEU  | CB   | 40.328     | 0.000       | .         |
| 1       | A     | 148 | LEU  | HB2  | 1.528      | 0.000       | .         |

*Continued on next page...*



*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 148 | LEU  | HB3  | 1.783      | 0.000       | .         |
| 1       | A     | 148 | LEU  | CG   | 28.864     | 0.000       | .         |
| 1       | A     | 148 | LEU  | HG   | 1.495      | 0.000       | .         |
| 1       | A     | 148 | LEU  | HD11 | 0.414      | 0.000       | .         |
| 1       | A     | 148 | LEU  | HD12 | 0.414      | 0.000       | .         |
| 1       | A     | 148 | LEU  | HD13 | 0.414      | 0.000       | .         |
| 1       | A     | 148 | LEU  | HD21 | 0.637      | 0.000       | .         |
| 1       | A     | 148 | LEU  | HD22 | 0.637      | 0.000       | .         |
| 1       | A     | 148 | LEU  | HD23 | 0.637      | 0.000       | .         |
| 1       | A     | 148 | LEU  | CD1  | 22.959     | 0.000       | .         |
| 1       | A     | 148 | LEU  | CD2  | 24.122     | 0.000       | .         |
| 1       | A     | 148 | LEU  | C    | 175.405    | 0.000       | .         |
| 1       | A     | 149 | THR  | N    | 116.934    | 0.000       | .         |
| 1       | A     | 149 | THR  | H    | 8.619      | 0.000       | .         |
| 1       | A     | 149 | THR  | CA   | 57.314     | 0.000       | .         |
| 1       | A     | 149 | THR  | HA   | 4.895      | 0.000       | .         |
| 1       | A     | 149 | THR  | CB   | 68.652     | 0.000       | .         |
| 1       | A     | 149 | THR  | HB   | 3.645      | 0.000       | .         |
| 1       | A     | 149 | THR  | HG21 | 0.567      | 0.001       | .         |
| 1       | A     | 149 | THR  | HG22 | 0.567      | 0.001       | .         |
| 1       | A     | 149 | THR  | HG23 | 0.567      | 0.001       | .         |
| 1       | A     | 149 | THR  | CG2  | 21.482     | 0.000       | .         |
| 1       | A     | 149 | THR  | C    | 172.075    | 0.006       | .         |
| 1       | A     | 150 | GLY  | N    | 115.314    | 0.000       | .         |
| 1       | A     | 150 | GLY  | H    | 8.683      | 0.000       | .         |
| 1       | A     | 150 | GLY  | CA   | 45.474     | 0.001       | .         |
| 1       | A     | 150 | GLY  | HA2  | 3.692      | 0.000       | .         |
| 1       | A     | 150 | GLY  | HA3  | 4.769      | 0.001       | .         |
| 1       | A     | 150 | GLY  | C    | 174.888    | 0.002       | .         |
| 1       | A     | 151 | ALA  | N    | 130.202    | 0.000       | .         |
| 1       | A     | 151 | ALA  | H    | 9.164      | 0.000       | .         |
| 1       | A     | 151 | ALA  | CA   | 50.063     | 0.000       | .         |
| 1       | A     | 151 | ALA  | HA   | 4.94       | 0.000       | .         |
| 1       | A     | 151 | ALA  | HB1  | 1.24       | 0.000       | .         |
| 1       | A     | 151 | ALA  | HB2  | 1.24       | 0.000       | .         |
| 1       | A     | 151 | ALA  | HB3  | 1.24       | 0.000       | .         |
| 1       | A     | 151 | ALA  | CB   | 18.59      | 0.000       | .         |
| 1       | A     | 151 | ALA  | C    | 176.447    | 0.000       | .         |
| 1       | A     | 152 | SER  | N    | 116.014    | 0.000       | .         |
| 1       | A     | 152 | SER  | H    | 8.411      | 0.000       | .         |
| 1       | A     | 152 | SER  | CA   | 63.345     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 152 | SER  | HA   | 3.776      | 0.000       | .         |
| 1       | A     | 152 | SER  | CB   | 62.321     | 0.000       | .         |
| 1       | A     | 152 | SER  | HB2  | 3.737      | 0.000       | .         |
| 1       | A     | 152 | SER  | HB3  | 3.813      | 0.000       | .         |
| 1       | A     | 152 | SER  | C    | 177.801    | 0.000       | .         |
| 1       | A     | 153 | ALA  | N    | 126.079    | 0.000       | .         |
| 1       | A     | 153 | ALA  | H    | 8.642      | 0.000       | .         |
| 1       | A     | 153 | ALA  | CA   | 55.523     | 0.000       | .         |
| 1       | A     | 153 | ALA  | HA   | 4.348      | 0.000       | .         |
| 1       | A     | 153 | ALA  | HB1  | 1.524      | 0.000       | .         |
| 1       | A     | 153 | ALA  | HB2  | 1.524      | 0.000       | .         |
| 1       | A     | 153 | ALA  | HB3  | 1.524      | 0.000       | .         |
| 1       | A     | 153 | ALA  | CB   | 18.163     | 0.001       | .         |
| 1       | A     | 153 | ALA  | C    | 180.574    | 0.000       | .         |
| 1       | A     | 154 | THR  | N    | 115.016    | 0.000       | .         |
| 1       | A     | 154 | THR  | H    | 7.876      | 0.000       | .         |
| 1       | A     | 154 | THR  | CA   | 65.504     | 0.000       | .         |
| 1       | A     | 154 | THR  | HA   | 4.092      | 0.000       | .         |
| 1       | A     | 154 | THR  | CB   | 68.601     | 0.000       | .         |
| 1       | A     | 154 | THR  | HB   | 4.159      | 0.000       | .         |
| 1       | A     | 154 | THR  | HG21 | 1.238      | 0.000       | .         |
| 1       | A     | 154 | THR  | HG22 | 1.238      | 0.000       | .         |
| 1       | A     | 154 | THR  | HG23 | 1.238      | 0.000       | .         |
| 1       | A     | 154 | THR  | CG2  | 22.157     | 0.000       | .         |
| 1       | A     | 154 | THR  | C    | 177.646    | 0.001       | .         |
| 1       | A     | 155 | ASP  | N    | 124.309    | 0.000       | .         |
| 1       | A     | 155 | ASP  | H    | 8.94       | 0.000       | .         |
| 1       | A     | 155 | ASP  | CA   | 58.312     | 0.000       | .         |
| 1       | A     | 155 | ASP  | HA   | 4.54       | 0.000       | .         |
| 1       | A     | 155 | ASP  | CB   | 39.988     | 0.000       | .         |
| 1       | A     | 155 | ASP  | HB2  | 2.628      | 0.000       | .         |
| 1       | A     | 155 | ASP  | HB3  | 2.753      | 0.000       | .         |
| 1       | A     | 155 | ASP  | C    | 179.23     | 0.000       | .         |
| 1       | A     | 156 | GLY  | N    | 106.804    | 0.000       | .         |
| 1       | A     | 156 | GLY  | H    | 8.468      | 0.000       | .         |
| 1       | A     | 156 | GLY  | CA   | 48.068     | 0.001       | .         |
| 1       | A     | 156 | GLY  | HA2  | 3.925      | 0.000       | .         |
| 1       | A     | 156 | GLY  | HA3  | 4.168      | 0.000       | .         |
| 1       | A     | 156 | GLY  | C    | 174.993    | 0.001       | .         |
| 1       | A     | 157 | ALA  | N    | 121.554    | 0.000       | .         |
| 1       | A     | 157 | ALA  | H    | 7.494      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 157 | ALA  | CA   | 55.349     | 0.000       | .         |
| 1       | A     | 157 | ALA  | HA   | 4.208      | 0.000       | .         |
| 1       | A     | 157 | ALA  | HB1  | 1.596      | 0.000       | .         |
| 1       | A     | 157 | ALA  | HB2  | 1.596      | 0.000       | .         |
| 1       | A     | 157 | ALA  | HB3  | 1.596      | 0.000       | .         |
| 1       | A     | 157 | ALA  | CB   | 18.001     | 0.000       | .         |
| 1       | A     | 157 | ALA  | C    | 180.332    | 0.000       | .         |
| 1       | A     | 158 | PHE  | N    | 120.341    | 0.000       | .         |
| 1       | A     | 158 | PHE  | H    | 7.421      | 0.000       | .         |
| 1       | A     | 158 | PHE  | CA   | 61.074     | 0.001       | .         |
| 1       | A     | 158 | PHE  | HA   | 4.357      | 0.000       | .         |
| 1       | A     | 158 | PHE  | CB   | 38.521     | 0.001       | .         |
| 1       | A     | 158 | PHE  | HB2  | 3.011      | 0.000       | .         |
| 1       | A     | 158 | PHE  | HB3  | 3.319      | 0.000       | .         |
| 1       | A     | 158 | PHE  | HD1  | 7.117      | 0.000       | .         |
| 1       | A     | 158 | PHE  | HD2  | 7.117      | 0.000       | .         |
| 1       | A     | 158 | PHE  | HE1  | 6.778      | 0.000       | .         |
| 1       | A     | 158 | PHE  | HE2  | 6.778      | 0.000       | .         |
| 1       | A     | 158 | PHE  | CD1  | 129.229    | 0.000       | .         |
| 1       | A     | 158 | PHE  | CE1  | 128.714    | 0.001       | .         |
| 1       | A     | 158 | PHE  | CE2  | 128.714    | 0.000       | .         |
| 1       | A     | 158 | PHE  | CD2  | 129.229    | 0.000       | .         |
| 1       | A     | 158 | PHE  | C    | 175.707    | 0.002       | .         |
| 1       | A     | 159 | TYR  | N    | 116.19     | 0.000       | .         |
| 1       | A     | 159 | TYR  | H    | 7.79       | 0.000       | .         |
| 1       | A     | 159 | TYR  | CA   | 62.938     | 0.000       | .         |
| 1       | A     | 159 | TYR  | HA   | 3.512      | 0.000       | .         |
| 1       | A     | 159 | TYR  | CB   | 39.879     | 0.000       | .         |
| 1       | A     | 159 | TYR  | HB2  | 2.791      | 0.000       | .         |
| 1       | A     | 159 | TYR  | HB3  | 2.924      | 0.000       | .         |
| 1       | A     | 159 | TYR  | HD1  | 7.147      | 0.000       | .         |
| 1       | A     | 159 | TYR  | HD2  | 7.147      | 0.000       | .         |
| 1       | A     | 159 | TYR  | HE1  | 7.147      | 0.000       | .         |
| 1       | A     | 159 | TYR  | HE2  | 7.147      | 0.000       | .         |
| 1       | A     | 159 | TYR  | HH   | 12.372     | 0.000       | .         |
| 1       | A     | 159 | TYR  | C    | 178.481    | 0.000       | .         |
| 1       | A     | 160 | ARG  | N    | 118.486    | 0.000       | .         |
| 1       | A     | 160 | ARG  | H    | 8.839      | 0.000       | .         |
| 1       | A     | 160 | ARG  | CA   | 58.641     | 0.000       | .         |
| 1       | A     | 160 | ARG  | HA   | 4.404      | 0.000       | .         |
| 1       | A     | 160 | ARG  | CB   | 29.948     | 0.001       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 160 | ARG  | HB2  | 1.761      | 0.000       | .         |
| 1       | A     | 160 | ARG  | HB3  | 1.85       | 0.000       | .         |
| 1       | A     | 160 | ARG  | CG   | 30.784     | 0.001       | .         |
| 1       | A     | 160 | ARG  | HG2  | 1.992      | 0.000       | .         |
| 1       | A     | 160 | ARG  | HG3  | 2.134      | 0.000       | .         |
| 1       | A     | 160 | ARG  | CD   | 43.899     | 0.000       | .         |
| 1       | A     | 160 | ARG  | HD2  | 3.227      | 0.000       | .         |
| 1       | A     | 160 | ARG  | HD3  | 3.404      | 0.000       | .         |
| 1       | A     | 160 | ARG  | NE   | 86.283     | 0.000       | .         |
| 1       | A     | 160 | ARG  | HE   | 7.216      | 0.000       | .         |
| 1       | A     | 160 | ARG  | C    | 179.885    | 0.000       | .         |
| 1       | A     | 161 | GLY  | N    | 109.979    | 0.000       | .         |
| 1       | A     | 161 | GLY  | H    | 7.814      | 0.000       | .         |
| 1       | A     | 161 | GLY  | CA   | 46.605     | 0.000       | .         |
| 1       | A     | 161 | GLY  | HA2  | 3.547      | 0.000       | .         |
| 1       | A     | 161 | GLY  | HA3  | 3.788      | 0.000       | .         |
| 1       | A     | 161 | GLY  | C    | 174.805    | 0.000       | .         |
| 1       | A     | 162 | LEU  | N    | 120.227    | 0.000       | .         |
| 1       | A     | 162 | LEU  | H    | 6.868      | 0.000       | .         |
| 1       | A     | 162 | LEU  | CA   | 56.404     | 0.000       | .         |
| 1       | A     | 162 | LEU  | HA   | 3.717      | 0.000       | .         |
| 1       | A     | 162 | LEU  | CB   | 42.284     | 0.000       | .         |
| 1       | A     | 162 | LEU  | HB2  | 0.106      | 0.000       | .         |
| 1       | A     | 162 | LEU  | HB3  | 0.481      | 0.000       | .         |
| 1       | A     | 162 | LEU  | CG   | 25.271     | 0.001       | .         |
| 1       | A     | 162 | LEU  | HG   | 0.536      | 0.000       | .         |
| 1       | A     | 162 | LEU  | HD11 | 0.148      | 0.000       | .         |
| 1       | A     | 162 | LEU  | HD12 | 0.148      | 0.000       | .         |
| 1       | A     | 162 | LEU  | HD13 | 0.148      | 0.000       | .         |
| 1       | A     | 162 | LEU  | HD21 | 0.06       | 0.000       | .         |
| 1       | A     | 162 | LEU  | HD22 | 0.06       | 0.000       | .         |
| 1       | A     | 162 | LEU  | HD23 | 0.06       | 0.000       | .         |
| 1       | A     | 162 | LEU  | CD1  | 23.776     | 0.000       | .         |
| 1       | A     | 162 | LEU  | CD2  | 24.685     | 0.000       | .         |
| 1       | A     | 162 | LEU  | C    | 178.59     | 0.000       | .         |
| 1       | A     | 163 | PHE  | N    | 113.675    | 0.001       | .         |
| 1       | A     | 163 | PHE  | H    | 8.031      | 0.000       | .         |
| 1       | A     | 163 | PHE  | CA   | 57.084     | 0.000       | .         |
| 1       | A     | 163 | PHE  | HA   | 4.879      | 0.000       | .         |
| 1       | A     | 163 | PHE  | CB   | 41.548     | 0.002       | .         |
| 1       | A     | 163 | PHE  | HB2  | 2.504      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 163 | PHE  | HB3  | 3.362      | 0.006       | .         |
| 1       | A     | 163 | PHE  | HD1  | 6.528      | 0.000       | .         |
| 1       | A     | 163 | PHE  | HD2  | 6.528      | 0.000       | .         |
| 1       | A     | 163 | PHE  | C    | 176.271    | 0.000       | .         |
| 1       | A     | 165 | ALA  | N    | 119.824    | 0.000       | .         |
| 1       | A     | 165 | ALA  | H    | 8.332      | 0.001       | .         |
| 1       | A     | 165 | ALA  | CA   | 55.023     | 0.000       | .         |
| 1       | A     | 165 | ALA  | HA   | 3.981      | 0.000       | .         |
| 1       | A     | 165 | ALA  | HB1  | 1.463      | 0.000       | .         |
| 1       | A     | 165 | ALA  | HB2  | 1.463      | 0.000       | .         |
| 1       | A     | 165 | ALA  | HB3  | 1.463      | 0.000       | .         |
| 1       | A     | 165 | ALA  | CB   | 19.318     | 0.000       | .         |
| 1       | A     | 165 | ALA  | C    | 177.803    | 0.002       | .         |
| 1       | A     | 166 | ASP  | N    | 113.029    | 0.000       | .         |
| 1       | A     | 166 | ASP  | H    | 8.38       | 0.000       | .         |
| 1       | A     | 166 | ASP  | CA   | 53.959     | 0.000       | .         |
| 1       | A     | 166 | ASP  | HA   | 4.64       | 0.001       | .         |
| 1       | A     | 166 | ASP  | CB   | 40.495     | 0.000       | .         |
| 1       | A     | 166 | ASP  | HB2  | 2.683      | 0.000       | .         |
| 1       | A     | 166 | ASP  | HB3  | 2.75       | 0.000       | .         |
| 1       | A     | 166 | ASP  | C    | 177.091    | 0.005       | .         |
| 1       | A     | 167 | PHE  | N    | 123.84     | 0.000       | .         |
| 1       | A     | 167 | PHE  | H    | 7.93       | 0.000       | .         |
| 1       | A     | 167 | PHE  | CA   | 60.141     | 0.000       | .         |
| 1       | A     | 167 | PHE  | HA   | 4.257      | 0.000       | .         |
| 1       | A     | 167 | PHE  | CB   | 39.855     | 0.001       | .         |
| 1       | A     | 167 | PHE  | HB2  | 3.082      | 0.000       | .         |
| 1       | A     | 167 | PHE  | HB3  | 3.33       | 0.000       | .         |
| 1       | A     | 167 | PHE  | HD1  | 7.262      | 0.000       | .         |
| 1       | A     | 167 | PHE  | HD2  | 7.262      | 0.000       | .         |
| 1       | A     | 167 | PHE  | CD1  | 133.043    | 0.002       | .         |
| 1       | A     | 167 | PHE  | CD2  | 133.043    | 0.000       | .         |
| 1       | A     | 167 | PHE  | C    | 175.402    | 0.000       | .         |
| 1       | A     | 169 | THR  | N    | 109.619    | 0.000       | .         |
| 1       | A     | 169 | THR  | H    | 7.613      | 0.000       | .         |
| 1       | A     | 169 | THR  | CA   | 61.577     | 0.000       | .         |
| 1       | A     | 169 | THR  | HA   | 4.506      | 0.000       | .         |
| 1       | A     | 169 | THR  | CB   | 70.911     | 0.000       | .         |
| 1       | A     | 169 | THR  | HB   | 4.287      | 0.000       | .         |
| 1       | A     | 169 | THR  | HG21 | 1.255      | 0.000       | .         |
| 1       | A     | 169 | THR  | HG22 | 1.255      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 169 | THR  | HG23 | 1.255      | 0.000       | .         |
| 1       | A     | 169 | THR  | CG2  | 21.6       | 0.000       | .         |
| 1       | A     | 169 | THR  | C    | 175.18     | 0.000       | .         |
| 1       | A     | 170 | GLU  | N    | 122.606    | 0.000       | .         |
| 1       | A     | 170 | GLU  | H    | 8.726      | 0.000       | .         |
| 1       | A     | 170 | GLU  | CA   | 56.926     | 0.000       | .         |
| 1       | A     | 170 | GLU  | HA   | 4.319      | 0.000       | .         |
| 1       | A     | 170 | GLU  | CB   | 29.9       | 0.003       | .         |
| 1       | A     | 170 | GLU  | HB2  | 1.955      | 0.000       | .         |
| 1       | A     | 170 | GLU  | HB3  | 2.11       | 0.000       | .         |
| 1       | A     | 170 | GLU  | CG   | 36.562     | 0.000       | .         |
| 1       | A     | 170 | GLU  | HG2  | 2.248      | 0.000       | .         |
| 1       | A     | 170 | GLU  | HG3  | 2.248      | 0.000       | .         |
| 1       | A     | 170 | GLU  | C    | 176.574    | 0.000       | .         |
| 1       | A     | 171 | SER  | N    | 116.348    | 0.000       | .         |
| 1       | A     | 171 | SER  | H    | 8.304      | 0.000       | .         |
| 1       | A     | 171 | SER  | CA   | 58.316     | 0.000       | .         |
| 1       | A     | 171 | SER  | HA   | 4.489      | 0.000       | .         |
| 1       | A     | 171 | SER  | CB   | 64.038     | 0.000       | .         |
| 1       | A     | 171 | SER  | HB2  | 3.814      | 0.000       | .         |
| 1       | A     | 171 | SER  | HB3  | 3.888      | 0.000       | .         |
| 1       | A     | 171 | SER  | C    | 175.071    | 0.000       | .         |
| 1       | A     | 172 | GLY  | N    | 110.804    | 0.000       | .         |
| 1       | A     | 172 | GLY  | H    | 8.442      | 0.000       | .         |
| 1       | A     | 172 | GLY  | CA   | 45.58      | 0.000       | .         |
| 1       | A     | 172 | GLY  | HA2  | 4.016      | 0.000       | .         |
| 1       | A     | 172 | GLY  | HA3  | 4.016      | 0.000       | .         |
| 1       | A     | 172 | GLY  | C    | 174.48     | 0.000       | .         |
| 1       | A     | 173 | THR  | N    | 112.852    | 0.001       | .         |
| 1       | A     | 173 | THR  | H    | 8.091      | 0.000       | .         |
| 1       | A     | 173 | THR  | CA   | 61.647     | 0.000       | .         |
| 1       | A     | 173 | THR  | HA   | 4.374      | 0.000       | .         |
| 1       | A     | 173 | THR  | CB   | 69.859     | 0.000       | .         |
| 1       | A     | 173 | THR  | HB   | 4.264      | 0.000       | .         |
| 1       | A     | 173 | THR  | HG21 | 1.161      | 0.000       | .         |
| 1       | A     | 173 | THR  | HG22 | 1.161      | 0.000       | .         |
| 1       | A     | 173 | THR  | HG23 | 1.161      | 0.000       | .         |
| 1       | A     | 173 | THR  | CG2  | 21.54      | 0.000       | .         |
| 1       | A     | 173 | THR  | C    | 174.561    | 0.000       | .         |
| 1       | A     | 174 | ASP  | N    | 122.678    | 0.000       | .         |
| 1       | A     | 174 | ASP  | H    | 8.41       | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 174 | ASP  | CA   | 54.558     | 0.000       | .         |
| 1       | A     | 174 | ASP  | HA   | 4.628      | 0.000       | .         |
| 1       | A     | 174 | ASP  | CB   | 41.226     | 0.000       | .         |
| 1       | A     | 174 | ASP  | HB2  | 2.692      | 0.000       | .         |
| 1       | A     | 174 | ASP  | HB3  | 2.692      | 0.000       | .         |
| 1       | A     | 174 | ASP  | C    | 176.68     | 0.000       | .         |
| 1       | A     | 176 | GLY  | N    | 108.87     | 0.000       | .         |
| 1       | A     | 176 | GLY  | H    | 8.373      | 0.000       | .         |
| 1       | A     | 176 | GLY  | CA   | 45.16      | 0.000       | .         |
| 1       | A     | 176 | GLY  | HA2  | 3.975      | 0.000       | .         |
| 1       | A     | 176 | GLY  | HA3  | 3.975      | 0.000       | .         |
| 1       | A     | 176 | GLY  | C    | 174.495    | 0.000       | .         |
| 1       | A     | 177 | GLY  | N    | 108.905    | 0.000       | .         |
| 1       | A     | 177 | GLY  | H    | 8.204      | 0.000       | .         |
| 1       | A     | 177 | GLY  | CA   | 44.722     | 0.000       | .         |
| 1       | A     | 177 | GLY  | HA2  | 3.999      | 0.000       | .         |
| 1       | A     | 177 | GLY  | HA3  | 3.999      | 0.000       | .         |
| 1       | A     | 177 | GLY  | C    | 174.063    | 0.000       | .         |
| 1       | A     | 178 | ARG  | N    | 121.089    | 0.000       | .         |
| 1       | A     | 178 | ARG  | H    | 8.48       | 0.000       | .         |
| 1       | A     | 178 | ARG  | CA   | 56.769     | 0.000       | .         |
| 1       | A     | 178 | ARG  | HA   | 4.507      | 0.000       | .         |
| 1       | A     | 178 | ARG  | CB   | 31.097     | 0.000       | .         |
| 1       | A     | 178 | ARG  | HB2  | 1.795      | 0.000       | .         |
| 1       | A     | 178 | ARG  | HB3  | 1.795      | 0.000       | .         |
| 1       | A     | 178 | ARG  | C    | 176.051    | 0.005       | .         |
| 1       | A     | 179 | ARG  | N    | 120.077    | 0.000       | .         |
| 1       | A     | 179 | ARG  | H    | 7.991      | 0.000       | .         |
| 1       | A     | 179 | ARG  | CA   | 54.157     | 0.000       | .         |
| 1       | A     | 179 | ARG  | HA   | 4.648      | 0.000       | .         |
| 1       | A     | 179 | ARG  | CB   | 32.38      | 0.000       | .         |
| 1       | A     | 179 | ARG  | HB2  | 1.604      | 0.000       | .         |
| 1       | A     | 179 | ARG  | HB3  | 1.936      | 0.000       | .         |
| 1       | A     | 179 | ARG  | CG   | 26.968     | 0.001       | .         |
| 1       | A     | 179 | ARG  | HG2  | 1.575      | 0.000       | .         |
| 1       | A     | 179 | ARG  | HG3  | 1.575      | 0.000       | .         |
| 1       | A     | 179 | ARG  | CD   | 43.353     | 0.000       | .         |
| 1       | A     | 179 | ARG  | HD2  | 3.14       | 0.000       | .         |
| 1       | A     | 179 | ARG  | HD3  | 3.22       | 0.000       | .         |
| 1       | A     | 179 | ARG  | NE   | 85.239     | 0.000       | .         |
| 1       | A     | 179 | ARG  | HE   | 7.192      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 179 | ARG  | C    | 174.905    | 0.000       | .         |
| 1       | A     | 180 | ALA  | N    | 123.062    | 0.000       | .         |
| 1       | A     | 180 | ALA  | H    | 8.603      | 0.000       | .         |
| 1       | A     | 180 | ALA  | CA   | 51.375     | 0.000       | .         |
| 1       | A     | 180 | ALA  | HA   | 4.623      | 0.000       | .         |
| 1       | A     | 180 | ALA  | HB1  | 1.358      | 0.000       | .         |
| 1       | A     | 180 | ALA  | HB2  | 1.358      | 0.000       | .         |
| 1       | A     | 180 | ALA  | HB3  | 1.358      | 0.000       | .         |
| 1       | A     | 180 | ALA  | CB   | 20.694     | 0.000       | .         |
| 1       | A     | 180 | ALA  | C    | 175.474    | 0.000       | .         |
| 1       | A     | 181 | ALA  | N    | 117.031    | 0.000       | .         |
| 1       | A     | 181 | ALA  | H    | 6.827      | 0.000       | .         |
| 1       | A     | 181 | ALA  | CA   | 50.805     | 0.000       | .         |
| 1       | A     | 181 | ALA  | HA   | 4.552      | 0.000       | .         |
| 1       | A     | 181 | ALA  | HB1  | 1.129      | 0.000       | .         |
| 1       | A     | 181 | ALA  | HB2  | 1.129      | 0.000       | .         |
| 1       | A     | 181 | ALA  | HB3  | 1.129      | 0.000       | .         |
| 1       | A     | 181 | ALA  | CB   | 23.205     | 0.000       | .         |
| 1       | A     | 181 | ALA  | C    | 174.519    | 0.000       | .         |
| 1       | A     | 182 | ILE  | N    | 119.999    | 0.001       | .         |
| 1       | A     | 182 | ILE  | H    | 8.611      | 0.000       | .         |
| 1       | A     | 182 | ILE  | CA   | 60.902     | 0.000       | .         |
| 1       | A     | 182 | ILE  | HA   | 4.454      | 0.000       | .         |
| 1       | A     | 182 | ILE  | CB   | 40.094     | 0.000       | .         |
| 1       | A     | 182 | ILE  | HB   | 1.623      | 0.000       | .         |
| 1       | A     | 182 | ILE  | HG21 | 0.669      | 0.000       | .         |
| 1       | A     | 182 | ILE  | HG22 | 0.669      | 0.000       | .         |
| 1       | A     | 182 | ILE  | HG23 | 0.669      | 0.000       | .         |
| 1       | A     | 182 | ILE  | CG2  | 17.231     | 0.000       | .         |
| 1       | A     | 182 | ILE  | CG1  | 26.711     | 0.000       | .         |
| 1       | A     | 182 | ILE  | HG12 | 1.386      | 0.000       | .         |
| 1       | A     | 182 | ILE  | HG13 | 1.386      | 0.000       | .         |
| 1       | A     | 182 | ILE  | HD11 | 0.992      | 0.000       | .         |
| 1       | A     | 182 | ILE  | HD12 | 0.992      | 0.000       | .         |
| 1       | A     | 182 | ILE  | HD13 | 0.992      | 0.000       | .         |
| 1       | A     | 182 | ILE  | CD1  | 13.608     | 0.000       | .         |
| 1       | A     | 182 | ILE  | C    | 174.733    | 0.000       | .         |
| 1       | A     | 183 | ARG  | N    | 126.472    | 0.000       | .         |
| 1       | A     | 183 | ARG  | H    | 9.519      | 0.000       | .         |
| 1       | A     | 183 | ARG  | CA   | 52.478     | 0.000       | .         |
| 1       | A     | 183 | ARG  | HA   | 4.588      | 0.001       | .         |

*Continued on next page...*



*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 183 | ARG  | CB   | 30.8       | 0.000       | .         |
| 1       | A     | 183 | ARG  | HB2  | 1.368      | 0.000       | .         |
| 1       | A     | 183 | ARG  | HB3  | 1.51       | 0.000       | .         |
| 1       | A     | 183 | ARG  | CG   | 25.904     | 0.000       | .         |
| 1       | A     | 183 | ARG  | HG2  | 1.3        | 0.000       | .         |
| 1       | A     | 183 | ARG  | HG3  | 1.193      | 0.000       | .         |
| 1       | A     | 183 | ARG  | CD   | 42.716     | 0.001       | .         |
| 1       | A     | 183 | ARG  | HD2  | 3.013      | 0.000       | .         |
| 1       | A     | 183 | ARG  | HD3  | 2.773      | 0.000       | .         |
| 1       | A     | 183 | ARG  | NE   | 88.73      | 0.000       | .         |
| 1       | A     | 183 | ARG  | HE   | 8.366      | 0.000       | .         |
| 1       | A     | 183 | ARG  | C    | 173.917    | 0.000       | .         |
| 1       | A     | 184 | GLN  | N    | 124.191    | 0.001       | .         |
| 1       | A     | 184 | GLN  | H    | 8.363      | 0.000       | .         |
| 1       | A     | 184 | GLN  | CA   | 54.76      | 0.000       | .         |
| 1       | A     | 184 | GLN  | HA   | 5.037      | 0.000       | .         |
| 1       | A     | 184 | GLN  | CB   | 28.12      | 0.005       | .         |
| 1       | A     | 184 | GLN  | HB2  | 1.921      | 0.000       | .         |
| 1       | A     | 184 | GLN  | HB3  | 2.021      | 0.000       | .         |
| 1       | A     | 184 | GLN  | CG   | 33.115     | 0.000       | .         |
| 1       | A     | 184 | GLN  | HG2  | 2.204      | 0.000       | .         |
| 1       | A     | 184 | GLN  | HG3  | 2.49       | 0.000       | .         |
| 1       | A     | 184 | GLN  | NE2  | 113.62     | 0.006       | .         |
| 1       | A     | 184 | GLN  | HE21 | 6.925      | 0.000       | .         |
| 1       | A     | 184 | GLN  | HE22 | 7.435      | 0.000       | .         |
| 1       | A     | 184 | GLN  | C    | 176.22     | 0.000       | .         |
| 1       | A     | 185 | VAL  | N    | 121.317    | 0.000       | .         |
| 1       | A     | 185 | VAL  | H    | 8.129      | 0.000       | .         |
| 1       | A     | 185 | VAL  | CA   | 59.32      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HA   | 4.653      | 0.000       | .         |
| 1       | A     | 185 | VAL  | CB   | 35.31      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HB   | 2.074      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HG11 | 0.564      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HG12 | 0.564      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HG13 | 0.564      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HG21 | 0.552      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HG22 | 0.552      | 0.000       | .         |
| 1       | A     | 185 | VAL  | HG23 | 0.552      | 0.000       | .         |
| 1       | A     | 185 | VAL  | CG1  | 17.532     | 0.000       | .         |
| 1       | A     | 185 | VAL  | CG2  | 21.665     | 0.000       | .         |
| 1       | A     | 185 | VAL  | C    | 175.72     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 186 | GLY  | N    | 106.792    | 0.000       | .         |
| 1       | A     | 186 | GLY  | H    | 8.272      | 0.000       | .         |
| 1       | A     | 186 | GLY  | CA   | 44.48      | 0.000       | .         |
| 1       | A     | 186 | GLY  | HA2  | 3.964      | 0.000       | .         |
| 1       | A     | 186 | GLY  | HA3  | 4.348      | 0.000       | .         |
| 1       | A     | 186 | GLY  | C    | 173.225    | 0.000       | .         |
| 1       | A     | 187 | PRO  | CD   | 49.756     | 0.000       | .         |
| 1       | A     | 187 | PRO  | CA   | 64.587     | 0.000       | .         |
| 1       | A     | 187 | PRO  | HA   | 4.392      | 0.000       | .         |
| 1       | A     | 187 | PRO  | CB   | 31.985     | 0.000       | .         |
| 1       | A     | 187 | PRO  | HB2  | 2.002      | 0.000       | .         |
| 1       | A     | 187 | PRO  | HB3  | 2.331      | 0.000       | .         |
| 1       | A     | 187 | PRO  | CG   | 27.202     | 0.000       | .         |
| 1       | A     | 187 | PRO  | HG2  | 2.002      | 0.000       | .         |
| 1       | A     | 187 | PRO  | HG3  | 2.002      | 0.000       | .         |
| 1       | A     | 187 | PRO  | HD2  | 3.676      | 0.000       | .         |
| 1       | A     | 187 | PRO  | HD3  | 3.676      | 0.000       | .         |
| 1       | A     | 187 | PRO  | C    | 177.272    | 0.000       | .         |
| 1       | A     | 188 | ALA  | N    | 120.342    | 0.000       | .         |
| 1       | A     | 188 | ALA  | H    | 8.396      | 0.000       | .         |
| 1       | A     | 188 | ALA  | CA   | 51.987     | 0.000       | .         |
| 1       | A     | 188 | ALA  | HA   | 4.426      | 0.000       | .         |
| 1       | A     | 188 | ALA  | HB1  | 1.408      | 0.000       | .         |
| 1       | A     | 188 | ALA  | HB2  | 1.408      | 0.000       | .         |
| 1       | A     | 188 | ALA  | HB3  | 1.408      | 0.000       | .         |
| 1       | A     | 188 | ALA  | CB   | 18.877     | 0.000       | .         |
| 1       | A     | 188 | ALA  | C    | 177.037    | 0.003       | .         |
| 1       | A     | 189 | ALA  | N    | 122.349    | 0.000       | .         |
| 1       | A     | 189 | ALA  | H    | 7.193      | 0.000       | .         |
| 1       | A     | 189 | ALA  | CA   | 50.235     | 0.000       | .         |
| 1       | A     | 189 | ALA  | HA   | 4.522      | 0.000       | .         |
| 1       | A     | 189 | ALA  | HB1  | 1.338      | 0.000       | .         |
| 1       | A     | 189 | ALA  | HB2  | 1.338      | 0.000       | .         |
| 1       | A     | 189 | ALA  | HB3  | 1.338      | 0.000       | .         |
| 1       | A     | 189 | ALA  | CB   | 18.74      | 0.000       | .         |
| 1       | A     | 189 | ALA  | C    | 174.753    | 0.000       | .         |
| 1       | A     | 191 | SER  | N    | 111.133    | 0.000       | .         |
| 1       | A     | 191 | SER  | H    | 8.091      | 0.000       | .         |
| 1       | A     | 191 | SER  | CA   | 56.539     | 0.000       | .         |
| 1       | A     | 191 | SER  | HA   | 4.989      | 0.000       | .         |
| 1       | A     | 191 | SER  | CB   | 66.627     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 191 | SER  | HB2  | 3.789      | 0.000       | .         |
| 1       | A     | 191 | SER  | HB3  | 3.927      | 0.000       | .         |
| 1       | A     | 191 | SER  | C    | 176.096    | 0.000       | .         |
| 1       | A     | 192 | GLY  | N    | 112.333    | 0.000       | .         |
| 1       | A     | 192 | GLY  | H    | 9.246      | 0.000       | .         |
| 1       | A     | 192 | GLY  | CA   | 43.54      | 0.000       | .         |
| 1       | A     | 192 | GLY  | HA2  | 2.844      | 0.000       | .         |
| 1       | A     | 192 | GLY  | HA3  | 4.397      | 0.000       | .         |
| 1       | A     | 192 | GLY  | C    | 171.9      | 0.000       | .         |
| 1       | A     | 193 | TRP  | N    | 118.721    | 0.000       | .         |
| 1       | A     | 193 | TRP  | H    | 9.063      | 0.000       | .         |
| 1       | A     | 193 | TRP  | CA   | 57.105     | 0.000       | .         |
| 1       | A     | 193 | TRP  | HA   | 4.9        | 0.000       | .         |
| 1       | A     | 193 | TRP  | CB   | 30.156     | 0.000       | .         |
| 1       | A     | 193 | TRP  | HB2  | 2.842      | 0.000       | .         |
| 1       | A     | 193 | TRP  | HB3  | 3.255      | 0.003       | .         |
| 1       | A     | 193 | TRP  | CD1  | 126.594    | 0.000       | .         |
| 1       | A     | 193 | TRP  | CE3  | 119.18     | 0.000       | .         |
| 1       | A     | 193 | TRP  | NE1  | 129.214    | 0.000       | .         |
| 1       | A     | 193 | TRP  | HD1  | 7.209      | 0.000       | .         |
| 1       | A     | 193 | TRP  | HE3  | 6.96       | 0.000       | .         |
| 1       | A     | 193 | TRP  | CZ3  | 120.926    | 0.004       | .         |
| 1       | A     | 193 | TRP  | CZ2  | 114.125    | 0.002       | .         |
| 1       | A     | 193 | TRP  | HE1  | 10.386     | 0.000       | .         |
| 1       | A     | 193 | TRP  | HZ3  | 6.78       | 0.001       | .         |
| 1       | A     | 193 | TRP  | CH2  | 122.776    | 0.006       | .         |
| 1       | A     | 193 | TRP  | HZ2  | 6.191      | 0.000       | .         |
| 1       | A     | 193 | TRP  | HH2  | 6.709      | 0.000       | .         |
| 1       | A     | 193 | TRP  | C    | 178.667    | 0.000       | .         |
| 1       | A     | 194 | TYR  | N    | 123.184    | 0.000       | .         |
| 1       | A     | 194 | TYR  | H    | 9.478      | 0.000       | .         |
| 1       | A     | 194 | TYR  | CA   | 56.022     | 0.000       | .         |
| 1       | A     | 194 | TYR  | HA   | 5.339      | 0.000       | .         |
| 1       | A     | 194 | TYR  | CB   | 40.878     | 0.000       | .         |
| 1       | A     | 194 | TYR  | HB2  | 2.696      | 0.000       | .         |
| 1       | A     | 194 | TYR  | HB3  | 3.043      | 0.000       | .         |
| 1       | A     | 194 | TYR  | HD1  | 7.043      | 0.000       | .         |
| 1       | A     | 194 | TYR  | HD2  | 7.043      | 0.000       | .         |
| 1       | A     | 194 | TYR  | HE1  | 6.463      | 0.000       | .         |
| 1       | A     | 194 | TYR  | HE2  | 6.463      | 0.000       | .         |
| 1       | A     | 194 | TYR  | CD1  | 133.511    | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 194 | TYR  | CE1  | 118.215    | 0.000       | .         |
| 1       | A     | 194 | TYR  | CE2  | 118.215    | 0.000       | .         |
| 1       | A     | 194 | TYR  | CD2  | 133.511    | 0.000       | .         |
| 1       | A     | 194 | TYR  | C    | 173.356    | 0.000       | .         |
| 1       | A     | 195 | PRO  | CD   | 51.081     | 0.000       | .         |
| 1       | A     | 195 | PRO  | CA   | 61.899     | 0.000       | .         |
| 1       | A     | 195 | PRO  | HA   | 4.841      | 0.000       | .         |
| 1       | A     | 195 | PRO  | CB   | 33.092     | 0.006       | .         |
| 1       | A     | 195 | PRO  | HB2  | 1.131      | 0.000       | .         |
| 1       | A     | 195 | PRO  | HB3  | 1.606      | 0.000       | .         |
| 1       | A     | 195 | PRO  | CG   | 26.762     | 0.007       | .         |
| 1       | A     | 195 | PRO  | HG2  | 1.468      | 0.000       | .         |
| 1       | A     | 195 | PRO  | HG3  | 1.728      | 0.000       | .         |
| 1       | A     | 195 | PRO  | HD2  | 4.077      | 0.000       | .         |
| 1       | A     | 195 | PRO  | HD3  | 4.077      | 0.000       | .         |
| 1       | A     | 195 | PRO  | C    | 174.534    | 0.000       | .         |
| 1       | A     | 196 | CYS  | N    | 117.655    | 0.000       | .         |
| 1       | A     | 196 | CYS  | H    | 8.481      | 0.000       | .         |
| 1       | A     | 196 | CYS  | CA   | 56.125     | 0.000       | .         |
| 1       | A     | 196 | CYS  | HA   | 5.37       | 0.000       | .         |
| 1       | A     | 196 | CYS  | CB   | 28.587     | 0.002       | .         |
| 1       | A     | 196 | CYS  | HB2  | 2.2        | 0.001       | .         |
| 1       | A     | 196 | CYS  | HB3  | 2.757      | 0.000       | .         |
| 1       | A     | 196 | CYS  | C    | 173.595    | 0.000       | .         |
| 1       | A     | 197 | PHE  | N    | 123.996    | 0.000       | .         |
| 1       | A     | 197 | PHE  | H    | 8.949      | 0.000       | .         |
| 1       | A     | 197 | PHE  | CA   | 56.151     | 0.008       | .         |
| 1       | A     | 197 | PHE  | HA   | 5.354      | 0.000       | .         |
| 1       | A     | 197 | PHE  | CB   | 42.742     | 0.001       | .         |
| 1       | A     | 197 | PHE  | HB2  | 2.422      | 0.000       | .         |
| 1       | A     | 197 | PHE  | HB3  | 2.578      | 0.000       | .         |
| 1       | A     | 197 | PHE  | HD1  | 6.971      | 0.000       | .         |
| 1       | A     | 197 | PHE  | HD2  | 6.971      | 0.000       | .         |
| 1       | A     | 197 | PHE  | HE1  | 6.307      | 0.000       | .         |
| 1       | A     | 197 | PHE  | HE2  | 6.307      | 0.000       | .         |
| 1       | A     | 197 | PHE  | CD1  | 131.873    | 0.006       | .         |
| 1       | A     | 197 | PHE  | CE1  | 129.201    | 0.000       | .         |
| 1       | A     | 197 | PHE  | CZ   | 128.95     | 0.001       | .         |
| 1       | A     | 197 | PHE  | HZ   | 5.747      | 0.001       | .         |
| 1       | A     | 197 | PHE  | CE2  | 129.201    | 0.000       | .         |
| 1       | A     | 197 | PHE  | CD2  | 131.873    | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 197 | PHE  | C    | 174.962    | 0.000       | .         |
| 1       | A     | 198 | ARG  | N    | 124.83     | 0.000       | .         |
| 1       | A     | 198 | ARG  | H    | 8.333      | 0.000       | .         |
| 1       | A     | 198 | ARG  | CA   | 57.465     | 0.000       | .         |
| 1       | A     | 198 | ARG  | HA   | 4.492      | 0.000       | .         |
| 1       | A     | 198 | ARG  | CB   | 30.263     | 0.000       | .         |
| 1       | A     | 198 | ARG  | HB2  | 1.887      | 0.000       | .         |
| 1       | A     | 198 | ARG  | HB3  | 1.887      | 0.000       | .         |
| 1       | A     | 198 | ARG  | CG   | 27.86      | 0.007       | .         |
| 1       | A     | 198 | ARG  | HG2  | 1.485      | 0.000       | .         |
| 1       | A     | 198 | ARG  | HG3  | 1.741      | 0.000       | .         |
| 1       | A     | 198 | ARG  | CD   | 42.735     | 0.008       | .         |
| 1       | A     | 198 | ARG  | HD2  | 2.968      | 0.000       | .         |
| 1       | A     | 198 | ARG  | HD3  | 3.148      | 0.000       | .         |
| 1       | A     | 198 | ARG  | C    | 176.261    | 0.000       | .         |
| 1       | A     | 199 | ALA  | N    | 128.106    | 0.000       | .         |
| 1       | A     | 199 | ALA  | H    | 8.991      | 0.000       | .         |
| 1       | A     | 199 | ALA  | CA   | 51.503     | 0.002       | .         |
| 1       | A     | 199 | ALA  | HA   | 4.955      | 0.000       | .         |
| 1       | A     | 199 | ALA  | HB1  | 1.511      | 0.000       | .         |
| 1       | A     | 199 | ALA  | HB2  | 1.511      | 0.000       | .         |
| 1       | A     | 199 | ALA  | HB3  | 1.511      | 0.000       | .         |
| 1       | A     | 199 | ALA  | CB   | 23.859     | 0.000       | .         |
| 1       | A     | 199 | ALA  | C    | 174.799    | 0.001       | .         |
| 1       | A     | 200 | GLN  | N    | 116.193    | 0.000       | .         |
| 1       | A     | 200 | GLN  | H    | 8.33       | 0.000       | .         |
| 1       | A     | 200 | GLN  | CA   | 54.537     | 0.000       | .         |
| 1       | A     | 200 | GLN  | HA   | 4.914      | 0.000       | .         |
| 1       | A     | 200 | GLN  | CB   | 31.218     | 0.000       | .         |
| 1       | A     | 200 | GLN  | HB2  | 2.07       | 0.000       | .         |
| 1       | A     | 200 | GLN  | HB3  | 2.296      | 0.000       | .         |
| 1       | A     | 200 | GLN  | CG   | 34.806     | 0.000       | .         |
| 1       | A     | 200 | GLN  | HG2  | 2.357      | 0.000       | .         |
| 1       | A     | 200 | GLN  | HG3  | 2.461      | 0.000       | .         |
| 1       | A     | 200 | GLN  | NE2  | 112.968    | 0.000       | .         |
| 1       | A     | 200 | GLN  | HE21 | 6.885      | 0.000       | .         |
| 1       | A     | 200 | GLN  | HE22 | 7.793      | 0.000       | .         |
| 1       | A     | 200 | GLN  | C    | 177.527    | 0.000       | .         |
| 1       | A     | 201 | GLU  | N    | 121.86     | 0.000       | .         |
| 1       | A     | 201 | GLU  | H    | 9.291      | 0.000       | .         |
| 1       | A     | 201 | GLU  | CA   | 60.587     | 0.001       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 201 | GLU  | HA   | 4.014      | 0.000       | .         |
| 1       | A     | 201 | GLU  | CB   | 29.148     | 0.000       | .         |
| 1       | A     | 201 | GLU  | HB2  | 2.135      | 0.000       | .         |
| 1       | A     | 201 | GLU  | HB3  | 2.135      | 0.000       | .         |
| 1       | A     | 201 | GLU  | CG   | 36.026     | 0.001       | .         |
| 1       | A     | 201 | GLU  | HG2  | 2.316      | 0.000       | .         |
| 1       | A     | 201 | GLU  | HG3  | 2.388      | 0.000       | .         |
| 1       | A     | 201 | GLU  | C    | 178.457    | 0.000       | .         |
| 1       | A     | 202 | SER  | N    | 112.055    | 0.000       | .         |
| 1       | A     | 202 | SER  | H    | 8.135      | 0.000       | .         |
| 1       | A     | 202 | SER  | CA   | 59.872     | 0.000       | .         |
| 1       | A     | 202 | SER  | HA   | 4.158      | 0.003       | .         |
| 1       | A     | 202 | SER  | CB   | 62.457     | 0.005       | .         |
| 1       | A     | 202 | SER  | HB2  | 3.882      | 0.000       | .         |
| 1       | A     | 202 | SER  | HB3  | 4.046      | 0.000       | .         |
| 1       | A     | 202 | SER  | C    | 175.178    | 0.000       | .         |
| 1       | A     | 203 | ALA  | N    | 125.841    | 0.000       | .         |
| 1       | A     | 203 | ALA  | H    | 8.448      | 0.000       | .         |
| 1       | A     | 203 | ALA  | CA   | 54.387     | 0.000       | .         |
| 1       | A     | 203 | ALA  | HA   | 4.219      | 0.000       | .         |
| 1       | A     | 203 | ALA  | HB1  | 1.559      | 0.000       | .         |
| 1       | A     | 203 | ALA  | HB2  | 1.559      | 0.000       | .         |
| 1       | A     | 203 | ALA  | HB3  | 1.559      | 0.000       | .         |
| 1       | A     | 203 | ALA  | CB   | 19.958     | 0.000       | .         |
| 1       | A     | 203 | ALA  | C    | 178.413    | 0.003       | .         |
| 1       | A     | 204 | VAL  | N    | 114.394    | 0.000       | .         |
| 1       | A     | 204 | VAL  | H    | 7.596      | 0.000       | .         |
| 1       | A     | 204 | VAL  | CA   | 68.475     | 0.000       | .         |
| 1       | A     | 204 | VAL  | HA   | 3.621      | 0.000       | .         |
| 1       | A     | 204 | VAL  | CB   | 28.71      | 0.000       | .         |
| 1       | A     | 204 | VAL  | HB   | 2.451      | 0.000       | .         |
| 1       | A     | 204 | VAL  | HG11 | 0.843      | 0.000       | .         |
| 1       | A     | 204 | VAL  | HG12 | 0.843      | 0.000       | .         |
| 1       | A     | 204 | VAL  | HG13 | 0.843      | 0.000       | .         |
| 1       | A     | 204 | VAL  | HG21 | 1.016      | 0.000       | .         |
| 1       | A     | 204 | VAL  | HG22 | 1.016      | 0.000       | .         |
| 1       | A     | 204 | VAL  | HG23 | 1.016      | 0.000       | .         |
| 1       | A     | 204 | VAL  | CG1  | 21.654     | 0.000       | .         |
| 1       | A     | 204 | VAL  | CG2  | 23.679     | 0.000       | .         |
| 1       | A     | 204 | VAL  | C    | 174.462    | 0.000       | .         |
| 1       | A     | 205 | PRO  | CD   | 49.304     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 205 | PRO  | CA   | 65.188     | 0.001       | .         |
| 1       | A     | 205 | PRO  | HA   | 4.261      | 0.000       | .         |
| 1       | A     | 205 | PRO  | CB   | 30.006     | 0.000       | .         |
| 1       | A     | 205 | PRO  | HB2  | 1.881      | 0.000       | .         |
| 1       | A     | 205 | PRO  | HB3  | 2.205      | 0.000       | .         |
| 1       | A     | 205 | PRO  | CG   | 27.632     | 0.000       | .         |
| 1       | A     | 205 | PRO  | HG2  | 1.988      | 0.000       | .         |
| 1       | A     | 205 | PRO  | HG3  | 2.14       | 0.000       | .         |
| 1       | A     | 205 | PRO  | HD2  | 3.495      | 0.000       | .         |
| 1       | A     | 205 | PRO  | HD3  | 4.076      | 0.000       | .         |
| 1       | A     | 205 | PRO  | C    | 179.755    | 0.000       | .         |
| 1       | A     | 207 | ALA  | N    | 120.649    | 0.000       | .         |
| 1       | A     | 207 | ALA  | H    | 8.42       | 0.000       | .         |
| 1       | A     | 207 | ALA  | CA   | 55.237     | 0.000       | .         |
| 1       | A     | 207 | ALA  | HA   | 3.884      | 0.000       | .         |
| 1       | A     | 207 | ALA  | HB1  | 1.467      | 0.000       | .         |
| 1       | A     | 207 | ALA  | HB2  | 1.467      | 0.000       | .         |
| 1       | A     | 207 | ALA  | HB3  | 1.467      | 0.000       | .         |
| 1       | A     | 207 | ALA  | CB   | 16.225     | 0.000       | .         |
| 1       | A     | 207 | ALA  | C    | 180.23     | 0.000       | .         |
| 1       | A     | 208 | VAL  | N    | 120.05     | 0.000       | .         |
| 1       | A     | 208 | VAL  | H    | 8.207      | 0.000       | .         |
| 1       | A     | 208 | VAL  | CA   | 65.533     | 0.000       | .         |
| 1       | A     | 208 | VAL  | HA   | 4.103      | 0.000       | .         |
| 1       | A     | 208 | VAL  | CB   | 31.94      | 0.006       | .         |
| 1       | A     | 208 | VAL  | HB   | 2.072      | 0.000       | .         |
| 1       | A     | 208 | VAL  | HG11 | 0.985      | 0.000       | .         |
| 1       | A     | 208 | VAL  | HG12 | 0.985      | 0.000       | .         |
| 1       | A     | 208 | VAL  | HG13 | 0.985      | 0.000       | .         |
| 1       | A     | 208 | VAL  | HG21 | 0.92       | 0.000       | .         |
| 1       | A     | 208 | VAL  | HG22 | 0.92       | 0.000       | .         |
| 1       | A     | 208 | VAL  | HG23 | 0.92       | 0.000       | .         |
| 1       | A     | 208 | VAL  | CG1  | 20.871     | 0.000       | .         |
| 1       | A     | 208 | VAL  | CG2  | 22.02      | 0.000       | .         |
| 1       | A     | 208 | VAL  | C    | 181.017    | 0.000       | .         |
| 1       | A     | 209 | MET  | N    | 122.465    | 0.001       | .         |
| 1       | A     | 209 | MET  | H    | 8.324      | 0.000       | .         |
| 1       | A     | 209 | MET  | CA   | 58.466     | 0.000       | .         |
| 1       | A     | 209 | MET  | HA   | 4.233      | 0.000       | .         |
| 1       | A     | 209 | MET  | CB   | 32.02      | 0.000       | .         |
| 1       | A     | 209 | MET  | HB2  | 2.226      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 209 | MET  | HB3  | 2.226      | 0.000       | .         |
| 1       | A     | 209 | MET  | CG   | 32.293     | 0.002       | .         |
| 1       | A     | 209 | MET  | HG2  | 2.632      | 0.000       | .         |
| 1       | A     | 209 | MET  | HG3  | 2.689      | 0.000       | .         |
| 1       | A     | 209 | MET  | C    | 178.138    | 0.000       | .         |
| 1       | A     | 210 | LEU  | N    | 118.186    | 0.000       | .         |
| 1       | A     | 210 | LEU  | H    | 7.454      | 0.000       | .         |
| 1       | A     | 210 | LEU  | CA   | 55.145     | 0.001       | .         |
| 1       | A     | 210 | LEU  | HA   | 4.358      | 0.000       | .         |
| 1       | A     | 210 | LEU  | CB   | 42.588     | 0.002       | .         |
| 1       | A     | 210 | LEU  | HB2  | 1.982      | 0.000       | .         |
| 1       | A     | 210 | LEU  | HB3  | 2.136      | 0.000       | .         |
| 1       | A     | 210 | LEU  | CG   | 26.696     | 0.000       | .         |
| 1       | A     | 210 | LEU  | HG   | 1.775      | 0.000       | .         |
| 1       | A     | 210 | LEU  | HD11 | 0.845      | 0.000       | .         |
| 1       | A     | 210 | LEU  | HD12 | 0.845      | 0.000       | .         |
| 1       | A     | 210 | LEU  | HD13 | 0.845      | 0.000       | .         |
| 1       | A     | 210 | LEU  | HD21 | 0.523      | 0.000       | .         |
| 1       | A     | 210 | LEU  | HD22 | 0.523      | 0.000       | .         |
| 1       | A     | 210 | LEU  | HD23 | 0.523      | 0.000       | .         |
| 1       | A     | 210 | LEU  | CD1  | 22.255     | 0.000       | .         |
| 1       | A     | 210 | LEU  | CD2  | 25.804     | 0.000       | .         |
| 1       | A     | 210 | LEU  | C    | 176.496    | 0.000       | .         |
| 1       | A     | 211 | GLY  | N    | 105.306    | 0.000       | .         |
| 1       | A     | 211 | GLY  | H    | 7.934      | 0.000       | .         |
| 1       | A     | 211 | GLY  | CA   | 44.971     | 0.000       | .         |
| 1       | A     | 211 | GLY  | HA2  | 3.754      | 0.000       | .         |
| 1       | A     | 211 | GLY  | HA3  | 4.421      | 0.000       | .         |
| 1       | A     | 211 | GLY  | C    | 174.824    | 0.000       | .         |
| 1       | A     | 212 | ALA  | N    | 123.929    | 0.000       | .         |
| 1       | A     | 212 | ALA  | H    | 8.52       | 0.000       | .         |
| 1       | A     | 212 | ALA  | CA   | 51.272     | 0.000       | .         |
| 1       | A     | 212 | ALA  | HA   | 4.727      | 0.000       | .         |
| 1       | A     | 212 | ALA  | HB1  | 1.199      | 0.000       | .         |
| 1       | A     | 212 | ALA  | HB2  | 1.199      | 0.000       | .         |
| 1       | A     | 212 | ALA  | HB3  | 1.199      | 0.000       | .         |
| 1       | A     | 212 | ALA  | CB   | 21.398     | 0.000       | .         |
| 1       | A     | 212 | ALA  | C    | 175.781    | 0.000       | .         |
| 1       | A     | 213 | SER  | N    | 111.856    | 0.000       | .         |
| 1       | A     | 213 | SER  | H    | 8.519      | 0.000       | .         |
| 1       | A     | 213 | SER  | CA   | 57.137     | 0.000       | .         |

*Continued on next page...*



*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 213 | SER  | HA   | 4.845      | 0.000       | .         |
| 1       | A     | 213 | SER  | CB   | 65.735     | 0.000       | .         |
| 1       | A     | 213 | SER  | HB2  | 3.631      | 0.000       | .         |
| 1       | A     | 213 | SER  | HB3  | 3.705      | 0.000       | .         |
| 1       | A     | 213 | SER  | C    | 173.076    | 0.000       | .         |
| 1       | A     | 214 | VAL  | N    | 123.846    | 0.000       | .         |
| 1       | A     | 214 | VAL  | H    | 8.796      | 0.000       | .         |
| 1       | A     | 214 | VAL  | CA   | 63.8       | 0.001       | .         |
| 1       | A     | 214 | VAL  | HA   | 3.921      | 0.000       | .         |
| 1       | A     | 214 | VAL  | CB   | 31.953     | 0.000       | .         |
| 1       | A     | 214 | VAL  | HB   | 1.894      | 0.000       | .         |
| 1       | A     | 214 | VAL  | HG11 | 0.707      | 0.000       | .         |
| 1       | A     | 214 | VAL  | HG12 | 0.707      | 0.000       | .         |
| 1       | A     | 214 | VAL  | HG13 | 0.707      | 0.000       | .         |
| 1       | A     | 214 | VAL  | HG21 | 0.748      | 0.000       | .         |
| 1       | A     | 214 | VAL  | HG22 | 0.748      | 0.000       | .         |
| 1       | A     | 214 | VAL  | HG23 | 0.748      | 0.000       | .         |
| 1       | A     | 214 | VAL  | CG1  | 21.196     | 0.000       | .         |
| 1       | A     | 214 | VAL  | CG2  | 21.237     | 0.000       | .         |
| 1       | A     | 214 | VAL  | C    | 176.385    | 0.001       | .         |
| 1       | A     | 215 | LEU  | N    | 127.468    | 0.000       | .         |
| 1       | A     | 215 | LEU  | H    | 9.414      | 0.000       | .         |
| 1       | A     | 215 | LEU  | CA   | 55.578     | 0.000       | .         |
| 1       | A     | 215 | LEU  | HA   | 4.448      | 0.000       | .         |
| 1       | A     | 215 | LEU  | CB   | 43.921     | 0.000       | .         |
| 1       | A     | 215 | LEU  | HB2  | 1.29       | 0.000       | .         |
| 1       | A     | 215 | LEU  | HB3  | 1.369      | 0.000       | .         |
| 1       | A     | 215 | LEU  | CG   | 26.425     | 0.000       | .         |
| 1       | A     | 215 | LEU  | HG   | 1.551      | 0.000       | .         |
| 1       | A     | 215 | LEU  | HD11 | 0.742      | 0.000       | .         |
| 1       | A     | 215 | LEU  | HD12 | 0.742      | 0.000       | .         |
| 1       | A     | 215 | LEU  | HD13 | 0.742      | 0.000       | .         |
| 1       | A     | 215 | LEU  | HD21 | 0.793      | 0.000       | .         |
| 1       | A     | 215 | LEU  | HD22 | 0.793      | 0.000       | .         |
| 1       | A     | 215 | LEU  | HD23 | 0.793      | 0.000       | .         |
| 1       | A     | 215 | LEU  | CD1  | 21.842     | 0.000       | .         |
| 1       | A     | 215 | LEU  | CD2  | 26.399     | 0.000       | .         |
| 1       | A     | 215 | LEU  | C    | 176.922    | 0.005       | .         |
| 1       | A     | 216 | LEU  | N    | 118.114    | 0.000       | .         |
| 1       | A     | 216 | LEU  | H    | 7.436      | 0.000       | .         |
| 1       | A     | 216 | LEU  | CA   | 55.173     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 216 | LEU  | HA   | 4.514      | 0.000       | .         |
| 1       | A     | 216 | LEU  | CB   | 45.698     | 0.008       | .         |
| 1       | A     | 216 | LEU  | HB2  | 1.427      | 0.000       | .         |
| 1       | A     | 216 | LEU  | HB3  | 1.461      | 0.000       | .         |
| 1       | A     | 216 | LEU  | CG   | 27.388     | 0.003       | .         |
| 1       | A     | 216 | LEU  | HG   | 1.581      | 0.000       | .         |
| 1       | A     | 216 | LEU  | HD11 | 1.07       | 0.000       | .         |
| 1       | A     | 216 | LEU  | HD12 | 1.07       | 0.000       | .         |
| 1       | A     | 216 | LEU  | HD13 | 1.07       | 0.000       | .         |
| 1       | A     | 216 | LEU  | HD21 | 0.794      | 0.000       | .         |
| 1       | A     | 216 | LEU  | HD22 | 0.794      | 0.000       | .         |
| 1       | A     | 216 | LEU  | HD23 | 0.794      | 0.000       | .         |
| 1       | A     | 216 | LEU  | CD1  | 23.304     | 0.002       | .         |
| 1       | A     | 216 | LEU  | CD2  | 26.471     | 0.000       | .         |
| 1       | A     | 216 | LEU  | C    | 173.002    | 0.003       | .         |
| 1       | A     | 217 | ARG  | N    | 125.403    | 0.001       | .         |
| 1       | A     | 217 | ARG  | H    | 8.408      | 0.000       | .         |
| 1       | A     | 217 | ARG  | CA   | 54.962     | 0.000       | .         |
| 1       | A     | 217 | ARG  | HA   | 5.421      | 0.000       | .         |
| 1       | A     | 217 | ARG  | CB   | 32.478     | 0.000       | .         |
| 1       | A     | 217 | ARG  | HB2  | 1.615      | 0.000       | .         |
| 1       | A     | 217 | ARG  | HB3  | 1.94       | 0.000       | .         |
| 1       | A     | 217 | ARG  | CG   | 28.543     | 0.000       | .         |
| 1       | A     | 217 | ARG  | HG2  | 1.55       | 0.000       | .         |
| 1       | A     | 217 | ARG  | HG3  | 1.55       | 0.000       | .         |
| 1       | A     | 217 | ARG  | CD   | 43.385     | 0.000       | .         |
| 1       | A     | 217 | ARG  | HD2  | 3.134      | 0.000       | .         |
| 1       | A     | 217 | ARG  | HD3  | 3.134      | 0.000       | .         |
| 1       | A     | 217 | ARG  | NE   | 85.449     | 0.001       | .         |
| 1       | A     | 217 | ARG  | HE   | 7.287      | 0.000       | .         |
| 1       | A     | 217 | ARG  | C    | 174.892    | 0.000       | .         |
| 1       | A     | 218 | TYR  | N    | 122.089    | 0.000       | .         |
| 1       | A     | 218 | TYR  | H    | 9.067      | 0.000       | .         |
| 1       | A     | 218 | TYR  | CA   | 56.306     | 0.000       | .         |
| 1       | A     | 218 | TYR  | HA   | 4.915      | 0.000       | .         |
| 1       | A     | 218 | TYR  | CB   | 39.749     | 0.008       | .         |
| 1       | A     | 218 | TYR  | HB2  | 2.836      | 0.000       | .         |
| 1       | A     | 218 | TYR  | HB3  | 3.085      | 0.000       | .         |
| 1       | A     | 218 | TYR  | HD1  | 6.61       | 0.000       | .         |
| 1       | A     | 218 | TYR  | HD2  | 6.61       | 0.000       | .         |
| 1       | A     | 218 | TYR  | HE1  | 6.468      | 0.003       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 218 | TYR  | HE2  | 6.468      | 0.003       | .         |
| 1       | A     | 218 | TYR  | CD1  | 132.93     | 0.000       | .         |
| 1       | A     | 218 | TYR  | CE1  | 118.252    | 0.000       | .         |
| 1       | A     | 218 | TYR  | CE2  | 118.252    | 0.002       | .         |
| 1       | A     | 218 | TYR  | CD2  | 132.93     | 0.000       | .         |
| 1       | A     | 218 | TYR  | C    | 171.774    | 0.004       | .         |
| 1       | A     | 219 | ASP  | N    | 118.737    | 0.001       | .         |
| 1       | A     | 219 | ASP  | H    | 8.557      | 0.000       | .         |
| 1       | A     | 219 | ASP  | CA   | 54.956     | 0.001       | .         |
| 1       | A     | 219 | ASP  | HA   | 4.992      | 0.000       | .         |
| 1       | A     | 219 | ASP  | CB   | 43.354     | 0.000       | .         |
| 1       | A     | 219 | ASP  | HB2  | 2.465      | 0.000       | .         |
| 1       | A     | 219 | ASP  | HB3  | 2.465      | 0.000       | .         |
| 1       | A     | 219 | ASP  | C    | 175.623    | 0.005       | .         |
| 1       | A     | 220 | CYS  | N    | 120.237    | 0.000       | .         |
| 1       | A     | 220 | CYS  | H    | 8.089      | 0.000       | .         |
| 1       | A     | 220 | CYS  | CA   | 56.956     | 0.000       | .         |
| 1       | A     | 220 | CYS  | HA   | 4.826      | 0.000       | .         |
| 1       | A     | 220 | CYS  | CB   | 27.85      | 0.001       | .         |
| 1       | A     | 220 | CYS  | HB2  | 2.762      | 0.001       | .         |
| 1       | A     | 220 | CYS  | HB3  | 3.327      | 0.000       | .         |
| 1       | A     | 220 | CYS  | C    | 174.069    | 0.000       | .         |
| 1       | A     | 221 | PRO  | CD   | 50.492     | 0.000       | .         |
| 1       | A     | 221 | PRO  | CA   | 65.45      | 0.000       | .         |
| 1       | A     | 221 | PRO  | HA   | 4.267      | 0.000       | .         |
| 1       | A     | 221 | PRO  | CB   | 31.817     | 0.000       | .         |
| 1       | A     | 221 | PRO  | HB2  | 1.854      | 0.000       | .         |
| 1       | A     | 221 | PRO  | HB3  | 2.402      | 0.000       | .         |
| 1       | A     | 221 | PRO  | CG   | 28.361     | 0.000       | .         |
| 1       | A     | 221 | PRO  | HG2  | 2.15       | 0.001       | .         |
| 1       | A     | 221 | PRO  | HG3  | 2.15       | 0.001       | .         |
| 1       | A     | 221 | PRO  | HD2  | 3.647      | 0.000       | .         |
| 1       | A     | 221 | PRO  | HD3  | 3.647      | 0.000       | .         |
| 1       | A     | 221 | PRO  | C    | 176.694    | 0.000       | .         |
| 1       | A     | 223 | GLY  | N    | 108.932    | 0.000       | .         |
| 1       | A     | 223 | GLY  | H    | 7.304      | 0.000       | .         |
| 1       | A     | 223 | GLY  | CA   | 45.09      | 0.000       | .         |
| 1       | A     | 223 | GLY  | HA2  | 4.375      | 0.001       | .         |
| 1       | A     | 223 | GLY  | HA3  | 3.854      | 0.000       | .         |
| 1       | A     | 223 | GLY  | C    | 169.416    | 0.000       | .         |
| 1       | A     | 225 | ALA  | N    | 124.14     | 0.001       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 225 | ALA  | H    | 8.807      | 0.000       | .         |
| 1       | A     | 225 | ALA  | CA   | 49.776     | 0.000       | .         |
| 1       | A     | 225 | ALA  | HA   | 5.198      | 0.000       | .         |
| 1       | A     | 225 | ALA  | HB1  | 0.195      | 0.000       | .         |
| 1       | A     | 225 | ALA  | HB2  | 0.195      | 0.000       | .         |
| 1       | A     | 225 | ALA  | HB3  | 0.195      | 0.000       | .         |
| 1       | A     | 225 | ALA  | CB   | 20.985     | 0.003       | .         |
| 1       | A     | 225 | ALA  | C    | 176.961    | 0.000       | .         |
| 1       | A     | 226 | VAL  | N    | 121.141    | 0.000       | .         |
| 1       | A     | 226 | VAL  | H    | 8.944      | 0.000       | .         |
| 1       | A     | 226 | VAL  | CA   | 61.008     | 0.000       | .         |
| 1       | A     | 226 | VAL  | HA   | 4.652      | 0.000       | .         |
| 1       | A     | 226 | VAL  | CB   | 34.647     | 0.000       | .         |
| 1       | A     | 226 | VAL  | HB   | 1.917      | 0.000       | .         |
| 1       | A     | 226 | VAL  | HG11 | 0.874      | 0.000       | .         |
| 1       | A     | 226 | VAL  | HG12 | 0.874      | 0.000       | .         |
| 1       | A     | 226 | VAL  | HG13 | 0.874      | 0.000       | .         |
| 1       | A     | 226 | VAL  | HG21 | 0.856      | 0.000       | .         |
| 1       | A     | 226 | VAL  | HG22 | 0.856      | 0.000       | .         |
| 1       | A     | 226 | VAL  | HG23 | 0.856      | 0.000       | .         |
| 1       | A     | 226 | VAL  | CG1  | 21.276     | 0.001       | .         |
| 1       | A     | 226 | VAL  | CG2  | 22.604     | 0.000       | .         |
| 1       | A     | 226 | VAL  | C    | 174.135    | 0.000       | .         |
| 1       | A     | 227 | VAL  | N    | 129.402    | 0.000       | .         |
| 1       | A     | 227 | VAL  | H    | 9.32       | 0.000       | .         |
| 1       | A     | 227 | VAL  | CA   | 62.21      | 0.000       | .         |
| 1       | A     | 227 | VAL  | HA   | 4.358      | 0.000       | .         |
| 1       | A     | 227 | VAL  | CB   | 31.937     | 0.000       | .         |
| 1       | A     | 227 | VAL  | HB   | 1.864      | 0.000       | .         |
| 1       | A     | 227 | VAL  | HG11 | 0.432      | 0.000       | .         |
| 1       | A     | 227 | VAL  | HG12 | 0.432      | 0.000       | .         |
| 1       | A     | 227 | VAL  | HG13 | 0.432      | 0.000       | .         |
| 1       | A     | 227 | VAL  | HG21 | 0.937      | 0.000       | .         |
| 1       | A     | 227 | VAL  | HG22 | 0.937      | 0.000       | .         |
| 1       | A     | 227 | VAL  | HG23 | 0.937      | 0.000       | .         |
| 1       | A     | 227 | VAL  | CG1  | 21.769     | 0.000       | .         |
| 1       | A     | 227 | VAL  | CG2  | 21.388     | 0.000       | .         |
| 1       | A     | 227 | VAL  | C    | 175.854    | 0.000       | .         |
| 1       | A     | 228 | VAL  | N    | 125.583    | 0.000       | .         |
| 1       | A     | 228 | VAL  | H    | 9.477      | 0.000       | .         |
| 1       | A     | 228 | VAL  | CA   | 59.499     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 228 | VAL  | HA   | 4.856      | 0.000       | .         |
| 1       | A     | 228 | VAL  | CB   | 34.749     | 0.000       | .         |
| 1       | A     | 228 | VAL  | HB   | 1.292      | 0.000       | .         |
| 1       | A     | 228 | VAL  | HG11 | 0.277      | 0.000       | .         |
| 1       | A     | 228 | VAL  | HG12 | 0.277      | 0.000       | .         |
| 1       | A     | 228 | VAL  | HG13 | 0.277      | 0.000       | .         |
| 1       | A     | 228 | VAL  | HG21 | 0.593      | 0.000       | .         |
| 1       | A     | 228 | VAL  | HG22 | 0.593      | 0.000       | .         |
| 1       | A     | 228 | VAL  | HG23 | 0.593      | 0.000       | .         |
| 1       | A     | 228 | VAL  | CG1  | 19.97      | 0.000       | .         |
| 1       | A     | 228 | VAL  | CG2  | 22.626     | 0.000       | .         |
| 1       | A     | 228 | VAL  | C    | 173.309    | 0.000       | .         |
| 1       | A     | 229 | SER  | N    | 115.241    | 0.001       | .         |
| 1       | A     | 229 | SER  | H    | 8.911      | 0.000       | .         |
| 1       | A     | 229 | SER  | CA   | 55.444     | 0.000       | .         |
| 1       | A     | 229 | SER  | HA   | 5.037      | 0.000       | .         |
| 1       | A     | 229 | SER  | CB   | 64.237     | 0.001       | .         |
| 1       | A     | 229 | SER  | HB2  | 3.651      | 0.001       | .         |
| 1       | A     | 229 | SER  | HB3  | 3.796      | 0.000       | .         |
| 1       | A     | 229 | SER  | C    | 173.303    | 0.000       | .         |
| 1       | A     | 230 | ALA  | N    | 128.38     | 0.000       | .         |
| 1       | A     | 230 | ALA  | H    | 9.272      | 0.000       | .         |
| 1       | A     | 230 | ALA  | CA   | 50.74      | 0.000       | .         |
| 1       | A     | 230 | ALA  | HA   | 3.906      | 0.000       | .         |
| 1       | A     | 230 | ALA  | HB1  | 1.32       | 0.000       | .         |
| 1       | A     | 230 | ALA  | HB2  | 1.32       | 0.000       | .         |
| 1       | A     | 230 | ALA  | HB3  | 1.32       | 0.000       | .         |
| 1       | A     | 230 | ALA  | CB   | 18.719     | 0.000       | .         |
| 1       | A     | 230 | ALA  | C    | 176.113    | 0.000       | .         |
| 1       | A     | 231 | PRO  | CD   | 49.864     | 0.001       | .         |
| 1       | A     | 231 | PRO  | CA   | 65.546     | 0.001       | .         |
| 1       | A     | 231 | PRO  | HA   | 4.039      | 0.000       | .         |
| 1       | A     | 231 | PRO  | CB   | 30.795     | 0.000       | .         |
| 1       | A     | 231 | PRO  | HB2  | 1.805      | 0.000       | .         |
| 1       | A     | 231 | PRO  | HB3  | 2.183      | 0.000       | .         |
| 1       | A     | 231 | PRO  | CG   | 27.796     | 0.001       | .         |
| 1       | A     | 231 | PRO  | HG2  | 1.74       | 0.000       | .         |
| 1       | A     | 231 | PRO  | HG3  | 1.74       | 0.000       | .         |
| 1       | A     | 231 | PRO  | HD2  | 3.735      | 0.000       | .         |
| 1       | A     | 231 | PRO  | HD3  | 3.735      | 0.000       | .         |
| 1       | A     | 231 | PRO  | C    | 178.14     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 232 | GLY  | N    | 103.872    | 0.000       | .         |
| 1       | A     | 232 | GLY  | H    | 8.357      | 0.000       | .         |
| 1       | A     | 232 | GLY  | CA   | 45.76      | 0.000       | .         |
| 1       | A     | 232 | GLY  | HA2  | 3.927      | 0.000       | .         |
| 1       | A     | 232 | GLY  | HA3  | 4.06       | 0.000       | .         |
| 1       | A     | 232 | GLY  | C    | 175.326    | 0.000       | .         |
| 1       | A     | 233 | GLY  | N    | 108.712    | 0.000       | .         |
| 1       | A     | 233 | GLY  | H    | 7.952      | 0.000       | .         |
| 1       | A     | 233 | GLY  | CA   | 44.755     | 0.000       | .         |
| 1       | A     | 233 | GLY  | HA2  | 3.495      | 0.000       | .         |
| 1       | A     | 233 | GLY  | HA3  | 4.483      | 0.000       | .         |
| 1       | A     | 233 | GLY  | C    | 174.359    | 0.000       | .         |
| 1       | A     | 234 | GLU  | N    | 124.033    | 0.000       | .         |
| 1       | A     | 234 | GLU  | H    | 9.852      | 0.000       | .         |
| 1       | A     | 234 | GLU  | CA   | 56.605     | 0.000       | .         |
| 1       | A     | 234 | GLU  | HA   | 4.78       | 0.000       | .         |
| 1       | A     | 234 | GLU  | CB   | 27.713     | 0.000       | .         |
| 1       | A     | 234 | GLU  | HB2  | 2.186      | 0.001       | .         |
| 1       | A     | 234 | GLU  | HB3  | 2.304      | 0.000       | .         |
| 1       | A     | 234 | GLU  | CG   | 35.335     | 0.000       | .         |
| 1       | A     | 234 | GLU  | HG2  | 2.645      | 0.001       | .         |
| 1       | A     | 234 | GLU  | HG3  | 2.645      | 0.001       | .         |
| 1       | A     | 234 | GLU  | C    | 173.219    | 0.002       | .         |
| 1       | A     | 235 | VAL  | N    | 121.051    | 0.000       | .         |
| 1       | A     | 235 | VAL  | H    | 8.552      | 0.000       | .         |
| 1       | A     | 235 | VAL  | CA   | 61.295     | 0.000       | .         |
| 1       | A     | 235 | VAL  | HA   | 5.566      | 0.000       | .         |
| 1       | A     | 235 | VAL  | CB   | 35.461     | 0.000       | .         |
| 1       | A     | 235 | VAL  | HB   | 2.124      | 0.000       | .         |
| 1       | A     | 235 | VAL  | HG11 | 0.419      | 0.000       | .         |
| 1       | A     | 235 | VAL  | HG12 | 0.419      | 0.000       | .         |
| 1       | A     | 235 | VAL  | HG13 | 0.419      | 0.000       | .         |
| 1       | A     | 235 | VAL  | HG21 | 1.029      | 0.000       | .         |
| 1       | A     | 235 | VAL  | HG22 | 1.029      | 0.000       | .         |
| 1       | A     | 235 | VAL  | HG23 | 1.029      | 0.000       | .         |
| 1       | A     | 235 | VAL  | CG1  | 22.968     | 0.000       | .         |
| 1       | A     | 235 | VAL  | CG2  | 21.895     | 0.000       | .         |
| 1       | A     | 235 | VAL  | C    | 175.611    | 0.001       | .         |
| 1       | A     | 236 | PHE  | N    | 121.141    | 0.000       | .         |
| 1       | A     | 236 | PHE  | H    | 8.893      | 0.000       | .         |
| 1       | A     | 236 | PHE  | CA   | 56.384     | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 236 | PHE  | HA   | 5.096      | 0.000       | .         |
| 1       | A     | 236 | PHE  | CB   | 41.634     | 0.000       | .         |
| 1       | A     | 236 | PHE  | HB2  | 3.171      | 0.000       | .         |
| 1       | A     | 236 | PHE  | HB3  | 3.348      | 0.000       | .         |
| 1       | A     | 236 | PHE  | HD1  | 7.524      | 0.000       | .         |
| 1       | A     | 236 | PHE  | HD2  | 7.524      | 0.000       | .         |
| 1       | A     | 236 | PHE  | HE1  | 7.424      | 0.000       | .         |
| 1       | A     | 236 | PHE  | HE2  | 7.424      | 0.000       | .         |
| 1       | A     | 236 | PHE  | CD1  | 132.919    | 0.001       | .         |
| 1       | A     | 236 | PHE  | CE1  | 130.755    | 0.000       | .         |
| 1       | A     | 236 | PHE  | CZ   | 128.323    | 0.000       | .         |
| 1       | A     | 236 | PHE  | HZ   | 7.079      | 0.000       | .         |
| 1       | A     | 236 | PHE  | CE2  | 130.755    | 0.000       | .         |
| 1       | A     | 236 | PHE  | CD2  | 132.919    | 0.000       | .         |
| 1       | A     | 236 | PHE  | C    | 170.306    | 0.000       | .         |
| 1       | A     | 237 | THR  | N    | 117.174    | 0.000       | .         |
| 1       | A     | 237 | THR  | H    | 9.187      | 0.000       | .         |
| 1       | A     | 237 | THR  | CA   | 61.401     | 0.000       | .         |
| 1       | A     | 237 | THR  | HA   | 5.284      | 0.000       | .         |
| 1       | A     | 237 | THR  | CB   | 70.037     | 0.000       | .         |
| 1       | A     | 237 | THR  | HB   | 4.358      | 0.000       | .         |
| 1       | A     | 237 | THR  | HG21 | 0.894      | 0.000       | .         |
| 1       | A     | 237 | THR  | HG22 | 0.894      | 0.000       | .         |
| 1       | A     | 237 | THR  | HG23 | 0.894      | 0.000       | .         |
| 1       | A     | 237 | THR  | CG2  | 24.15      | 0.005       | .         |
| 1       | A     | 237 | THR  | C    | 173.97     | 0.002       | .         |
| 1       | A     | 238 | LEU  | N    | 126.937    | 0.000       | .         |
| 1       | A     | 238 | LEU  | H    | 9.396      | 0.000       | .         |
| 1       | A     | 238 | LEU  | CA   | 52.89      | 0.000       | .         |
| 1       | A     | 238 | LEU  | HA   | 5.202      | 0.000       | .         |
| 1       | A     | 238 | LEU  | CB   | 44.325     | 0.000       | .         |
| 1       | A     | 238 | LEU  | HB2  | 1.187      | 0.000       | .         |
| 1       | A     | 238 | LEU  | HB3  | 1.93       | 0.000       | .         |
| 1       | A     | 238 | LEU  | CG   | 26.368     | 0.001       | .         |
| 1       | A     | 238 | LEU  | HG   | 1.923      | 0.000       | .         |
| 1       | A     | 238 | LEU  | HD11 | 1.24       | 0.000       | .         |
| 1       | A     | 238 | LEU  | HD12 | 1.24       | 0.000       | .         |
| 1       | A     | 238 | LEU  | HD13 | 1.24       | 0.000       | .         |
| 1       | A     | 238 | LEU  | HD21 | 0.762      | 0.000       | .         |
| 1       | A     | 238 | LEU  | HD22 | 0.762      | 0.000       | .         |
| 1       | A     | 238 | LEU  | HD23 | 0.762      | 0.000       | .         |

*Continued on next page...*

*Continued from previous page...*

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 238 | LEU  | CD1  | 25.564     | 0.000       | .         |
| 1       | A     | 238 | LEU  | CD2  | 26.61      | 0.000       | .         |
| 1       | A     | 238 | LEU  | C    | 174.624    | 0.000       | .         |
| 1       | A     | 239 | LEU  | N    | 125.653    | 0.000       | .         |
| 1       | A     | 239 | LEU  | H    | 8.65       | 0.000       | .         |
| 1       | A     | 239 | LEU  | CA   | 53.058     | 0.000       | .         |
| 1       | A     | 239 | LEU  | HA   | 4.842      | 0.000       | .         |
| 1       | A     | 239 | LEU  | CB   | 43.662     | 0.000       | .         |
| 1       | A     | 239 | LEU  | HB2  | 1.011      | 0.000       | .         |
| 1       | A     | 239 | LEU  | HB3  | 1.517      | 0.000       | .         |
| 1       | A     | 239 | LEU  | CG   | 27.283     | 0.000       | .         |
| 1       | A     | 239 | LEU  | HG   | 1.213      | 0.000       | .         |
| 1       | A     | 239 | LEU  | HD11 | 0.551      | 0.000       | .         |
| 1       | A     | 239 | LEU  | HD12 | 0.551      | 0.000       | .         |
| 1       | A     | 239 | LEU  | HD13 | 0.551      | 0.000       | .         |
| 1       | A     | 239 | LEU  | HD21 | 0.638      | 0.000       | .         |
| 1       | A     | 239 | LEU  | HD22 | 0.638      | 0.000       | .         |
| 1       | A     | 239 | LEU  | HD23 | 0.638      | 0.000       | .         |
| 1       | A     | 239 | LEU  | CD1  | 23.813     | 0.000       | .         |
| 1       | A     | 239 | LEU  | CD2  | 25.194     | 0.000       | .         |
| 1       | A     | 239 | LEU  | C    | 176.05     | 0.000       | .         |
| 1       | A     | 240 | LEU  | N    | 126.147    | 0.000       | .         |
| 1       | A     | 240 | LEU  | H    | 8.772      | 0.000       | .         |
| 1       | A     | 240 | LEU  | CA   | 54.12      | 0.000       | .         |
| 1       | A     | 240 | LEU  | HA   | 4.86       | 0.000       | .         |
| 1       | A     | 240 | LEU  | CB   | 39.782     | 0.000       | .         |
| 1       | A     | 240 | LEU  | HB2  | 1.168      | 0.000       | .         |
| 1       | A     | 240 | LEU  | HB3  | 1.918      | 0.000       | .         |
| 1       | A     | 240 | LEU  | CG   | 26.434     | 0.000       | .         |
| 1       | A     | 240 | LEU  | HG   | 1.591      | 0.000       | .         |
| 1       | A     | 240 | LEU  | HD11 | 0.58       | 0.000       | .         |
| 1       | A     | 240 | LEU  | HD12 | 0.58       | 0.000       | .         |
| 1       | A     | 240 | LEU  | HD13 | 0.58       | 0.000       | .         |
| 1       | A     | 240 | LEU  | HD21 | 0.827      | 0.000       | .         |
| 1       | A     | 240 | LEU  | HD22 | 0.827      | 0.000       | .         |
| 1       | A     | 240 | LEU  | HD23 | 0.827      | 0.000       | .         |
| 1       | A     | 240 | LEU  | CD1  | 23.362     | 0.000       | .         |
| 1       | A     | 240 | LEU  | CD2  | 25.714     | 0.000       | .         |
| 1       | A     | 240 | LEU  | C    | 177.332    | 0.000       | .         |
| 1       | A     | 241 | THR  | N    | 114.683    | 0.000       | .         |
| 1       | A     | 241 | THR  | H    | 8.35       | 0.000       | .         |

*Continued on next page...*



Continued from previous page...

| List ID | Chain | Res | Type | Atom | Shift Data |             |           |
|---------|-------|-----|------|------|------------|-------------|-----------|
|         |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1       | A     | 241 | THR  | CA   | 61.603     | 0.000       | .         |
| 1       | A     | 241 | THR  | HA   | 4.43       | 0.000       | .         |
| 1       | A     | 241 | THR  | CB   | 70.544     | 0.000       | .         |
| 1       | A     | 241 | THR  | HB   | 4.192      | 0.000       | .         |
| 1       | A     | 241 | THR  | HG21 | 1.093      | 0.000       | .         |
| 1       | A     | 241 | THR  | HG22 | 1.093      | 0.000       | .         |
| 1       | A     | 241 | THR  | HG23 | 1.093      | 0.000       | .         |
| 1       | A     | 241 | THR  | CG2  | 20.804     | 0.000       | .         |
| 1       | A     | 241 | THR  | C    | 174.119    | 0.000       | .         |
| 1       | A     | 242 | ASP  | N    | 128.315    | 0.000       | .         |
| 1       | A     | 242 | ASP  | H    | 8.125      | 0.000       | .         |
| 1       | A     | 242 | ASP  | CA   | 56.157     | 0.001       | .         |
| 1       | A     | 242 | ASP  | HA   | 4.484      | 0.000       | .         |
| 1       | A     | 242 | ASP  | CB   | 42.615     | 0.000       | .         |
| 1       | A     | 242 | ASP  | HB2  | 2.463      | 0.000       | .         |
| 1       | A     | 242 | ASP  | HB3  | 2.714      | 0.000       | .         |
| 1       | A     | 242 | ASP  | C    | 180.403    | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H1   | 3.722      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H2   | 6.735      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H3   | 6.197      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H4   | 6.016      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H5   | 2.129      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H6   | 1.352      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H7   | 5.998      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | Q24  | 2.435      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | Q26  | 0.737      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | Q27  | 0.573      | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H13  | 12.835     | 0.000       | .         |
| 1       | A     | 301 | WOZ  | H14  | 10.192     | 0.000       | .         |

### 7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

| Nucleus                | # values | Correction $\pm$ precision, ppm | Suggested action           |
|------------------------|----------|---------------------------------|----------------------------|
| $^{13}\text{C}_\alpha$ | 241      | $0.06 \pm 0.30$                 | None needed ( $< 0.5$ ppm) |
| $^{13}\text{C}_\beta$  | 205      | $0.61 \pm 0.65$                 | None needed (imprecise)    |
| $^{13}\text{C}'$       | 220      | $0.47 \pm 0.34$                 | None needed ( $< 0.5$ ppm) |
| $^{15}\text{N}$        | 217      | $0.65 \pm 0.89$                 | None needed (imprecise)    |

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

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 96 atoms were assigned a chemical shift out of a possible 2500. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total        | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|--------------|----------------|-----------------|-----------------|
| Backbone  | 53/983 (5%)  | 22/406 (5%)    | 22/394 (6%)     | 9/183 (5%)      |
| Sidechain | 43/1317 (3%) | 30/874 (3%)    | 13/403 (3%)     | 0/40 (0%)       |
| Aromatic  | 0/200 (0%)   | 0/97 (0%)      | 0/97 (0%)       | 0/6 (0%)        |
| Overall   | 96/2500 (4%) | 52/1377 (4%)   | 35/894 (4%)     | 9/229 (4%)      |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 5%, i.e. 140 atoms were assigned a chemical shift out of a possible 3006. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total         | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|---------------|----------------|-----------------|-----------------|
| Backbone  | 82/1225 (7%)  | 34/508 (7%)    | 34/490 (7%)     | 14/227 (6%)     |
| Sidechain | 56/1550 (4%)  | 39/1023 (4%)   | 17/478 (4%)     | 0/49 (0%)       |
| Aromatic  | 2/231 (1%)    | 1/114 (1%)     | 1/108 (1%)      | 0/9 (0%)        |
| Overall   | 140/3006 (5%) | 74/1645 (4%)   | 52/1076 (5%)    | 14/285 (5%)     |

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

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

| List Id | Chain | Res | Type | Atom | Shift, ppm | Expected range, ppm | Z-score |
|---------|-------|-----|------|------|------------|---------------------|---------|
| 1       | A     | 147 | LEU  | HB2  | -1.79      | -0.07 – 3.30        | -10.1   |
| 1       | A     | 18  | LEU  | HB2  | -1.65      | -0.07 – 3.30        | -9.7    |
| 1       | A     | 147 | LEU  | HB3  | -1.79      | -0.26 – 3.31        | -9.3    |
| 1       | A     | 18  | LEU  | HB3  | -0.96      | -0.26 – 3.31        | -7.0    |
| 1       | A     | 34  | PHE  | HB2  | 1.15       | 1.20 – 4.80         | -5.1    |

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray

bars.

Random coil index (RCI) for chain A:

