



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 01:02 AM BST

PDB ID : 2LEJ  
Title : human prion protein mutant HuPrP(90-231, M129, V210I)  
Authors : Biljan, I.; Ilc, G.; Giachin, G.; Raspadori, A.; Zhukov, I.; Plavec, J.; Legname, G.  
Deposited on : 2011-06-16

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

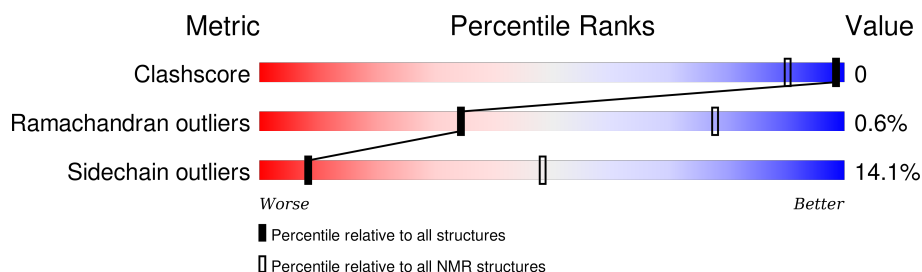
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



| Metric                | Whole archive<br>(#Entries) | NMR archive<br>(#Entries) |
|-----------------------|-----------------------------|---------------------------|
| Clashscore            | 114402                      | 11133                     |
| Ramachandran outliers | 111179                      | 9975                      |
| Sidechain outliers    | 111093                      | 9958                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 147    |                  |

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

| Well-defined (core) protein residues |                                  |                   |              |
|--------------------------------------|----------------------------------|-------------------|--------------|
| Well-defined core                    | Residue range (total)            | Backbone RMSD (Å) | Medoid model |
| 1                                    | A:117-A:165, A:172-A:220<br>(98) | 0.24              | 15           |

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 4 clusters and 5 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2254 atoms, of which 1091 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

| Mol | Chain | Residues | Atoms |     |      |     |     |    | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|----|-------|
| 1   | A     | 147      | Total | C   | H    | N   | O   | S  | 0     |
|     |       |          | 2254  | 715 | 1091 | 209 | 227 | 12 |       |

There are 6 discrepancies between the modelled and reference sequences:

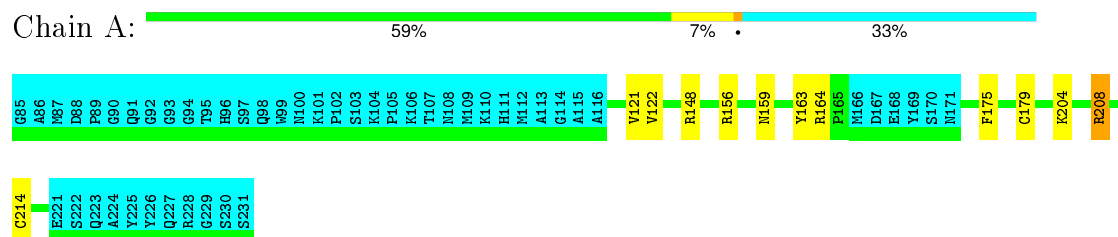
| Chain | Residue | Modelled | Actual | Comment             | Reference  |
|-------|---------|----------|--------|---------------------|------------|
| A     | 85      | GLY      | -      | EXPRESSION TAG      | UNP P04156 |
| A     | 86      | ALA      | -      | EXPRESSION TAG      | UNP P04156 |
| A     | 87      | MET      | -      | EXPRESSION TAG      | UNP P04156 |
| A     | 88      | ASP      | -      | EXPRESSION TAG      | UNP P04156 |
| A     | 89      | PRO      | -      | EXPRESSION TAG      | UNP P04156 |
| A     | 210     | ILE      | VAL    | ENGINEERED MUTATION | UNP P04156 |

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

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

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

- Molecule 1: Major prion protein

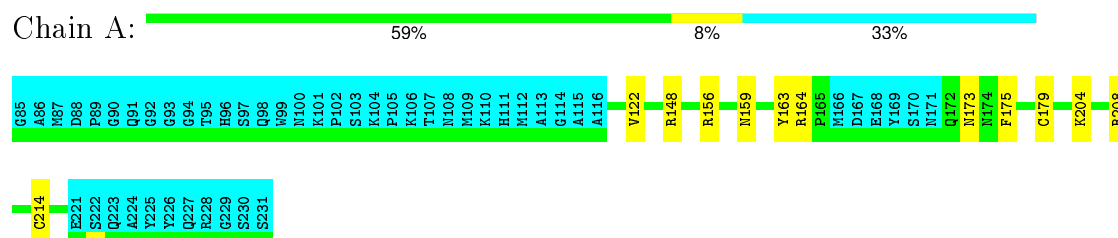


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

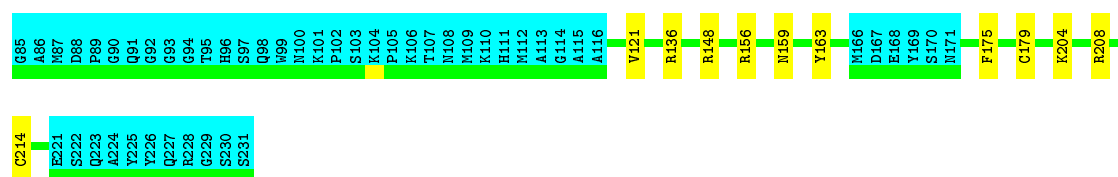
- Molecule 1: Major prion protein



#### 4.2.2 Score per residue for model 2

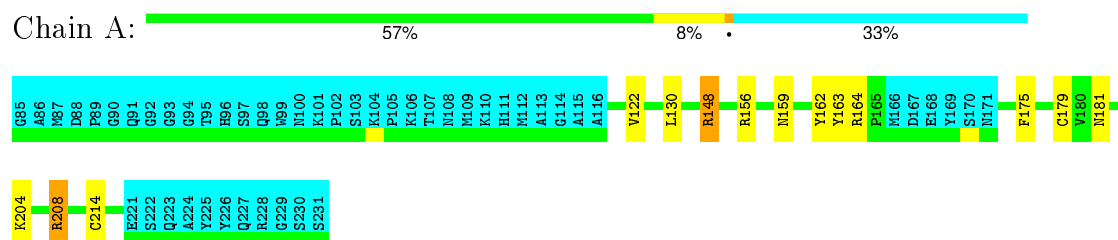
- Molecule 1: Major prion protein





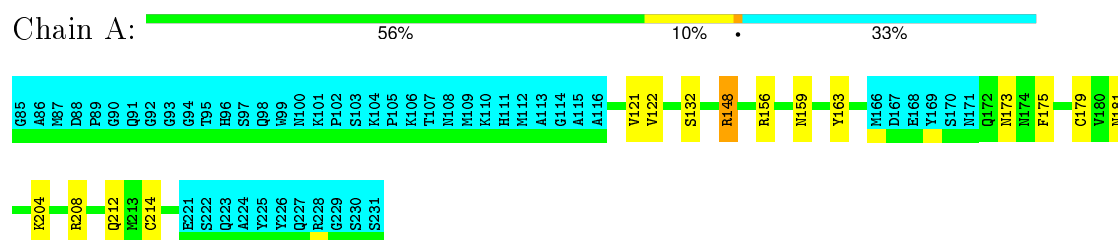
### 4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



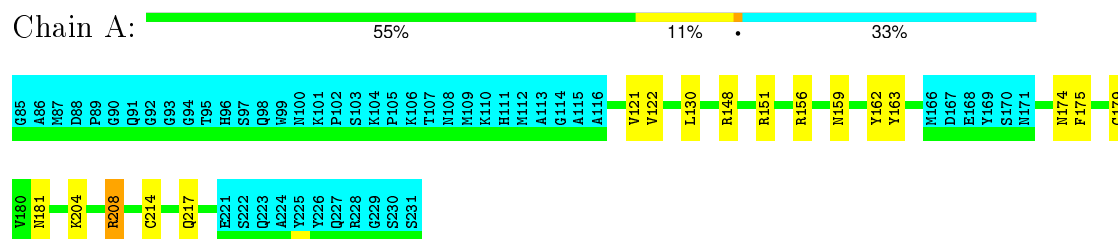
#### 4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



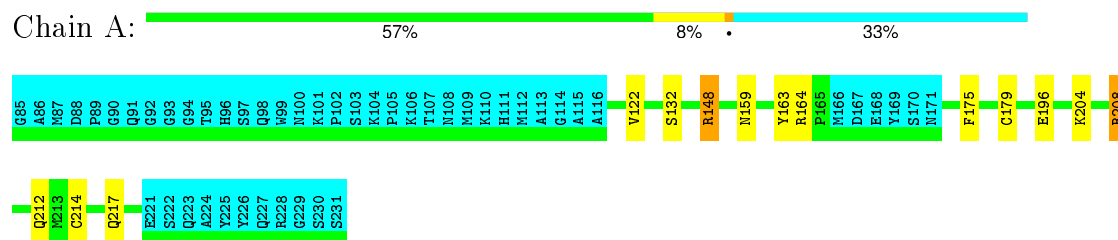
#### 4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



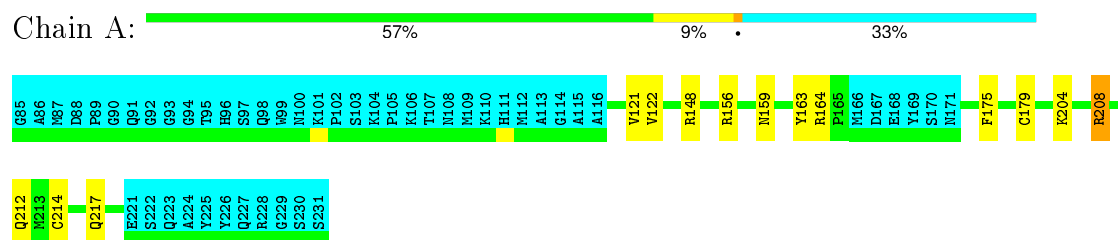
#### 4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



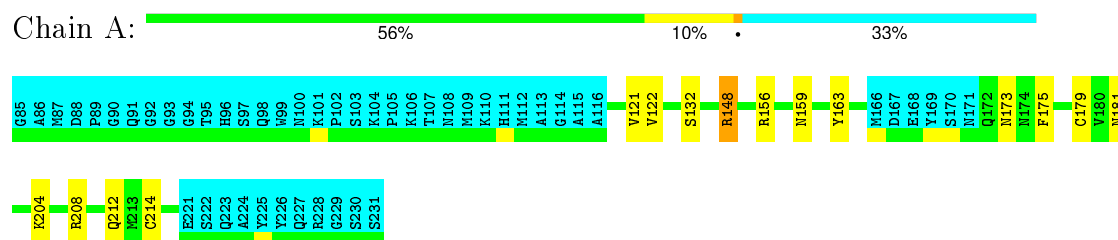
#### 4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



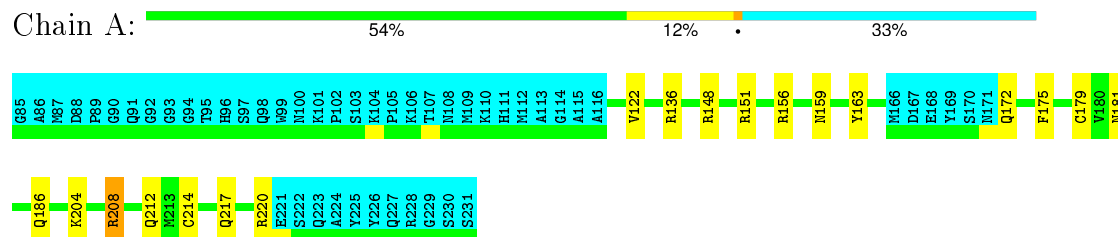
#### 4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



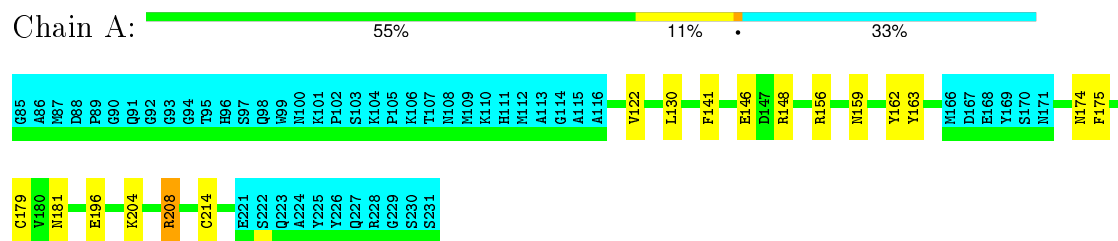
#### 4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



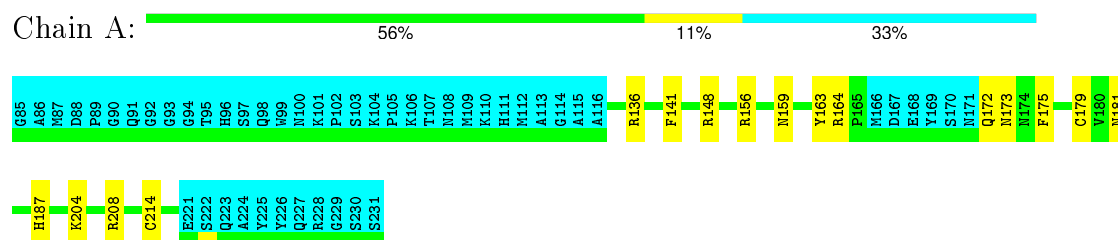
#### 4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



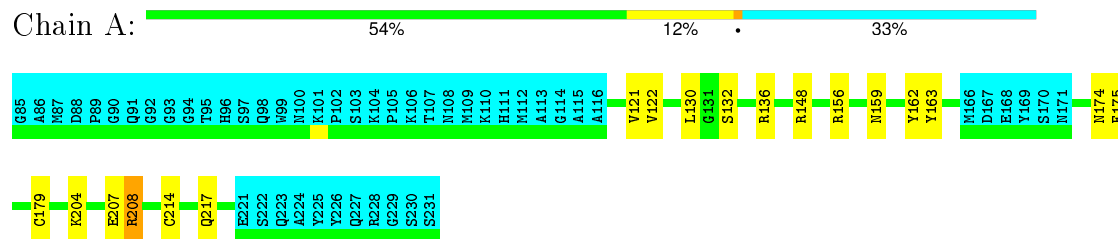
#### 4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



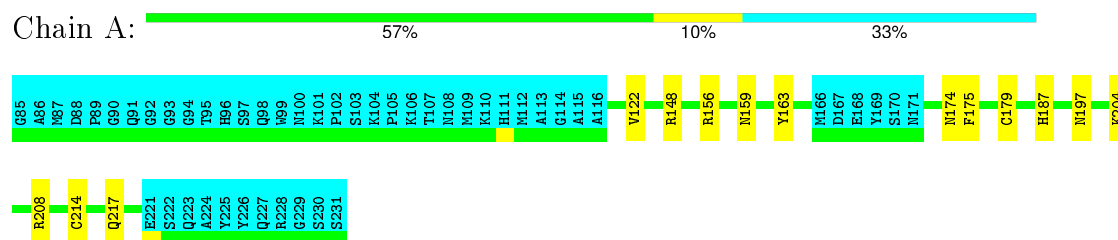
#### 4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



#### 4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein





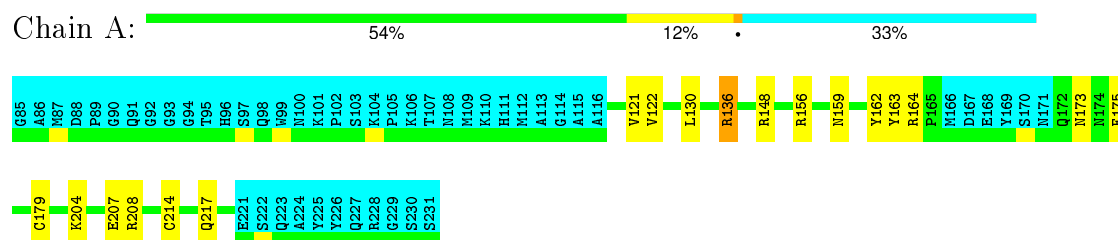
#### 4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



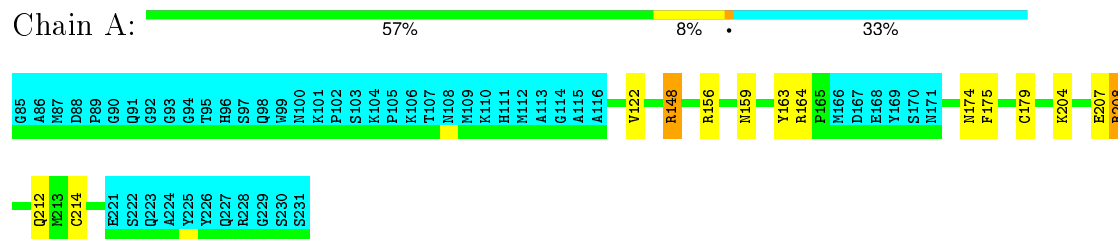
#### 4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Major prion protein



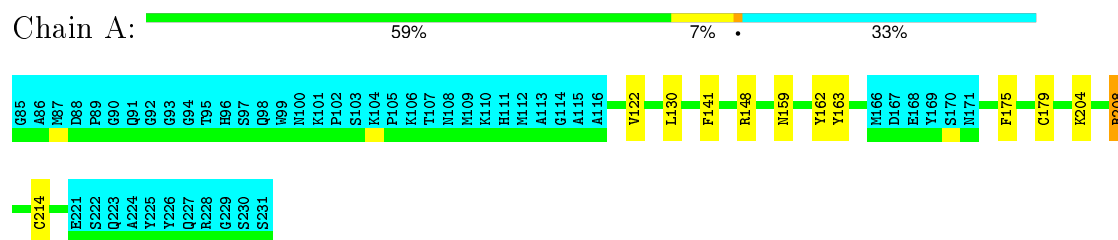
#### 4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



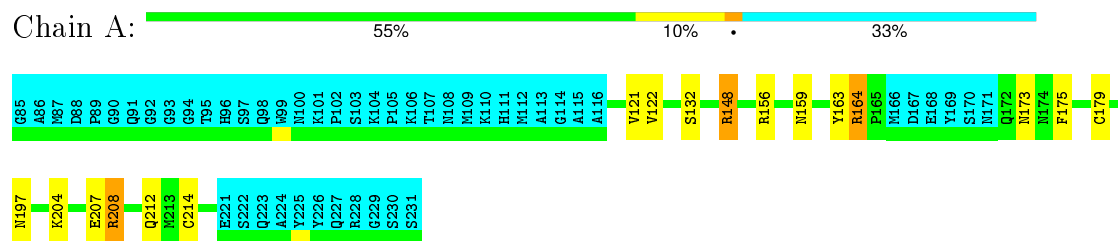
#### 4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



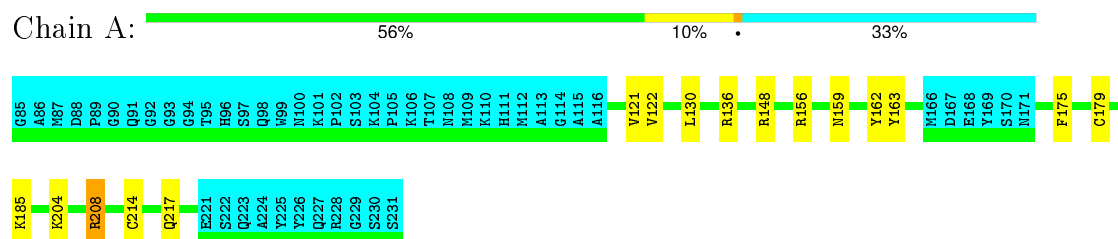
#### 4.2.18 Score per residue for model 18

- Molecule 1: Major prion protein



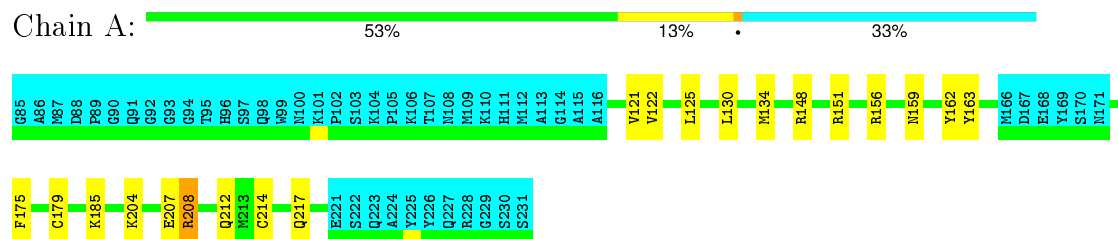
#### 4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein



#### 4.2.20 Score per residue for model 20

- Molecule 1: Major prion protein



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

| Software name | Classification     | Version |
|---------------|--------------------|---------|
| CYANA         | structure solution | 3.0     |
| YASARA        | refinement         | 11.5.22 |

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)                       | 2lej_cs.str |
| Number of chemical shift lists               | 1           |
| Total number of shifts                       | 1536        |
| Number of shifts mapped to atoms             | 0           |
| Number of unparsed shifts                    | 1536        |
| Number of shifts with mapping errors         | 0           |
| Number of shifts with mapping warnings       | 0           |
| Assignment completeness (well-defined parts) | 0%          |

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

## 6 Model quality [i](#)

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

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

| Mol | Chain | Bond lengths |                    | Bond angles |                     |
|-----|-------|--------------|--------------------|-------------|---------------------|
|     |       | RMSZ         | #Z>5               | RMSZ        | #Z>5                |
| 1   | A     | 0.69±0.01    | 0±0/813 (0.0±0.0%) | 0.74±0.02   | 3±1/1099 (0.3±0.1%) |
| All | All   | 0.69         | 0/16260 (0.0%)     | 0.74        | 60/21980 (0.3%)     |

There are no bond-length outliers.

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

| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) | Models |       |
|-----|-------|-----|------|-----------|------|-------------|----------|--------|-------|
|     |       |     |      |           |      |             |          | Worst  | Total |
| 1   | A     | 151 | ARG  | NE-CZ-NH1 | 6.79 | 123.70      | 120.30   | 9      | 3     |
| 1   | A     | 208 | ARG  | NE-CZ-NH1 | 6.29 | 123.45      | 120.30   | 9      | 13    |
| 1   | A     | 164 | ARG  | NE-CZ-NH1 | 6.07 | 123.34      | 120.30   | 1      | 9     |
| 1   | A     | 148 | ARG  | NE-CZ-NH1 | 6.04 | 123.32      | 120.30   | 9      | 13    |
| 1   | A     | 156 | ARG  | NE-CZ-NH1 | 5.65 | 123.12      | 120.30   | 2      | 16    |
| 1   | A     | 136 | ARG  | NE-CZ-NH1 | 5.61 | 123.10      | 120.30   | 15     | 5     |
| 1   | A     | 220 | ARG  | NE-CZ-NH1 | 5.08 | 122.84      | 120.30   | 9      | 1     |

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     | 795   | 756      | 756      | 0±1     |
| All | All   | 15900 | 15120    | 15120    | 10      |

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 0.

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

| Atom-1           | Atom-2          | Clash(Å) | Distance(Å) | Models |       |
|------------------|-----------------|----------|-------------|--------|-------|
|                  |                 |          |             | Worst  | Total |
| 1:A:130:LEU:HD13 | 1:A:162:TYR:CE2 | 0.52     | 2.38        | 14     | 9     |
| 1:A:180:VAL:HG11 | 1:A:211:GLU:HA  | 0.42     | 1.92        | 14     | 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     | 98/147 (67%)    | 91±1 (92±1%) | 7±1 (7±1%) | 1±0 (1±1%) | 34          | 78 |
| All | All   | 1960/2940 (67%) | 1813 (92%)   | 136 (7%)   | 11 (1%)    | 34          | 78 |

All 1 unique Ramachandran outliers are listed below.

| Mol | Chain | Res | Type | Models (Total) |
|-----|-------|-----|------|----------------|
| 1   | A     | 121 | VAL  | 11             |

### 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     | 86/123 (70%)    | 74±2 (86±2%) | 12±2 (14±2%) | 8           | 48 |
| All | All   | 1720/2460 (70%) | 1478 (86%)   | 242 (14%)    | 8           | 48 |

All 29 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     | 159 | ASN  | 20             |
| 1   | A     | 204 | LYS  | 20             |
| 1   | A     | 214 | CYS  | 20             |
| 1   | A     | 175 | PHE  | 20             |
| 1   | A     | 163 | TYR  | 20             |
| 1   | A     | 208 | ARG  | 20             |
| 1   | A     | 179 | CYS  | 20             |
| 1   | A     | 122 | VAL  | 18             |
| 1   | A     | 148 | ARG  | 14             |
| 1   | A     | 217 | GLN  | 10             |
| 1   | A     | 212 | GLN  | 8              |
| 1   | A     | 181 | ASN  | 7              |
| 1   | A     | 173 | ASN  | 7              |
| 1   | A     | 207 | GLU  | 5              |
| 1   | A     | 174 | ASN  | 5              |
| 1   | A     | 132 | SER  | 5              |
| 1   | A     | 141 | PHE  | 3              |
| 1   | A     | 136 | ARG  | 3              |
| 1   | A     | 156 | ARG  | 2              |
| 1   | A     | 187 | HIS  | 2              |
| 1   | A     | 197 | ASN  | 2              |
| 1   | A     | 185 | LYS  | 2              |
| 1   | A     | 172 | GLN  | 2              |
| 1   | A     | 196 | GLU  | 2              |
| 1   | A     | 146 | GLU  | 1              |
| 1   | A     | 125 | LEU  | 1              |
| 1   | A     | 186 | GLN  | 1              |
| 1   | A     | 164 | ARG  | 1              |
| 1   | A     | 134 | MET  | 1              |

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2lej\_cs.str

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

#### 7.1.1 Bookkeeping

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

|   |      |
|---|------|
| Total number of shifts                  | 1536 |
| Number of shifts mapped to atoms        | 0    |
| Number of unparsed shifts               | 1536 |
| Number of shifts with mapping errors    | 0    |
| Number of shifts with mapping warnings  | 0    |
| Number of shift outliers (ShiftChecker) | 0    |

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

- Entity instance (chain) must be specified. All 1536 occurrences are reported below.

| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1        | .     | 86  | ALA  | H    | 8.614      | 0.02        | 1         |
| 2        | .     | 86  | ALA  | HA   | 4.295      | 0.02        | 1         |
| 3        | .     | 86  | ALA  | HB   | 1.380      | 0.02        | 1         |
| 4        | .     | 86  | ALA  | HB   | 1.380      | 0.02        | 1         |
| 5        | .     | 86  | ALA  | HB   | 1.380      | 0.02        | 1         |
| 6        | .     | 86  | ALA  | CA   | 52.649     | 0.20        | 1         |
| 7        | .     | 86  | ALA  | CB   | 19.285     | 0.20        | 1         |
| 8        | .     | 86  | ALA  | N    | 123.505    | 0.20        | 1         |
| 9        | .     | 87  | MET  | H    | 8.448      | 0.02        | 1         |
| 10       | .     | 87  | MET  | HA   | 4.464      | 0.02        | 1         |
| 11       | .     | 87  | MET  | HB2  | 2.064      | 0.02        | 2         |
| 12       | .     | 87  | MET  | HB3  | 1.961      | 0.02        | 2         |
| 13       | .     | 87  | MET  | HG2  | 2.563      | 0.02        | 2         |
| 14       | .     | 87  | MET  | HG3  | 2.491      | 0.02        | 2         |
| 15       | .     | 87  | MET  | HE   | 2.006      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 16       | .     | 87  | MET  | HE   | 2.006      | 0.02        | 1         |
| 17       | .     | 87  | MET  | HE   | 2.006      | 0.02        | 1         |
| 18       | .     | 87  | MET  | CA   | 55.143     | 0.20        | 1         |
| 19       | .     | 87  | MET  | CB   | 32.762     | 0.20        | 1         |
| 20       | .     | 87  | MET  | CG   | 32.096     | 0.20        | 1         |
| 21       | .     | 87  | MET  | CE   | 17.736     | 0.20        | 1         |
| 22       | .     | 87  | MET  | N    | 118.564    | 0.20        | 1         |
| 23       | .     | 88  | ASP  | H    | 8.191      | 0.02        | 1         |
| 24       | .     | 88  | ASP  | HA   | 4.850      | 0.02        | 1         |
| 25       | .     | 88  | ASP  | HB2  | 2.719      | 0.02        | 2         |
| 26       | .     | 88  | ASP  | HB3  | 2.578      | 0.02        | 2         |
| 27       | .     | 88  | ASP  | CA   | 52.357     | 0.20        | 1         |
| 28       | .     | 88  | ASP  | CB   | 41.147     | 0.20        | 1         |
| 29       | .     | 88  | ASP  | N    | 123.158    | 0.20        | 1         |
| 30       | .     | 89  | PRO  | HA   | 4.416      | 0.02        | 1         |
| 31       | .     | 89  | PRO  | HB2  | 2.281      | 0.02        | 2         |
| 32       | .     | 89  | PRO  | HB3  | 1.880      | 0.02        | 2         |
| 33       | .     | 89  | PRO  | HG2  | 2.015      | 0.02        | 2         |
| 34       | .     | 89  | PRO  | HG3  | 2.015      | 0.02        | 2         |
| 35       | .     | 89  | PRO  | HD2  | 3.785      | 0.02        | 2         |
| 36       | .     | 89  | PRO  | HD3  | 3.785      | 0.02        | 2         |
| 37       | .     | 89  | PRO  | CA   | 63.841     | 0.20        | 1         |
| 38       | .     | 89  | PRO  | CB   | 32.054     | 0.20        | 1         |
| 39       | .     | 89  | PRO  | CG   | 27.343     | 0.20        | 1         |
| 40       | .     | 89  | PRO  | CD   | 50.833     | 0.20        | 1         |
| 41       | .     | 90  | GLY  | H    | 8.513      | 0.02        | 1         |
| 42       | .     | 90  | GLY  | HA2  | 3.930      | 0.02        | 2         |
| 43       | .     | 90  | GLY  | HA3  | 3.930      | 0.02        | 2         |
| 44       | .     | 90  | GLY  | CA   | 45.314     | 0.20        | 1         |
| 45       | .     | 90  | GLY  | N    | 108.575    | 0.20        | 1         |
| 46       | .     | 91  | GLN  | H    | 8.121      | 0.02        | 1         |
| 47       | .     | 91  | GLN  | HA   | 4.336      | 0.02        | 1         |
| 48       | .     | 91  | GLN  | HB2  | 2.169      | 0.02        | 2         |
| 49       | .     | 91  | GLN  | HB3  | 1.989      | 0.02        | 2         |
| 50       | .     | 91  | GLN  | HG2  | 2.364      | 0.02        | 2         |
| 51       | .     | 91  | GLN  | HG3  | 2.353      | 0.02        | 2         |
| 52       | .     | 91  | GLN  | CA   | 56.009     | 0.20        | 1         |
| 53       | .     | 91  | GLN  | CB   | 29.329     | 0.20        | 1         |
| 54       | .     | 91  | GLN  | CG   | 33.837     | 0.20        | 1         |
| 55       | .     | 91  | GLN  | N    | 119.514    | 0.20        | 1         |
| 56       | .     | 92  | GLY  | H    | 8.463      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 57       | .     | 92  | GLY  | HA2  | 3.977      | 0.02        | 2         |
| 58       | .     | 92  | GLY  | HA3  | 3.977      | 0.02        | 2         |
| 59       | .     | 92  | GLY  | CA   | 45.320     | 0.20        | 1         |
| 60       | .     | 92  | GLY  | N    | 109.760    | 0.20        | 1         |
| 61       | .     | 93  | GLY  | H    | 8.306      | 0.02        | 1         |
| 62       | .     | 93  | GLY  | HA2  | 4.013      | 0.02        | 2         |
| 63       | .     | 93  | GLY  | HA3  | 3.934      | 0.02        | 2         |
| 64       | .     | 93  | GLY  | CA   | 45.346     | 0.20        | 1         |
| 65       | .     | 93  | GLY  | N    | 108.709    | 0.20        | 1         |
| 66       | .     | 94  | GLY  | H    | 8.312      | 0.02        | 1         |
| 67       | .     | 94  | GLY  | HA2  | 3.978      | 0.02        | 2         |
| 68       | .     | 94  | GLY  | HA3  | 3.978      | 0.02        | 2         |
| 69       | .     | 94  | GLY  | CA   | 45.364     | 0.20        | 1         |
| 70       | .     | 94  | GLY  | N    | 108.696    | 0.20        | 1         |
| 71       | .     | 95  | THR  | H    | 8.096      | 0.02        | 1         |
| 72       | .     | 95  | THR  | HA   | 4.272      | 0.02        | 1         |
| 73       | .     | 95  | THR  | HB   | 4.164      | 0.02        | 1         |
| 74       | .     | 95  | THR  | HG2  | 1.147      | 0.02        | 1         |
| 75       | .     | 95  | THR  | HG2  | 1.147      | 0.02        | 1         |
| 76       | .     | 95  | THR  | HG2  | 1.147      | 0.02        | 1         |
| 77       | .     | 95  | THR  | CA   | 62.079     | 0.20        | 1         |
| 78       | .     | 95  | THR  | CB   | 69.520     | 0.20        | 1         |
| 79       | .     | 95  | THR  | CG2  | 21.548     | 0.20        | 1         |
| 80       | .     | 95  | THR  | N    | 113.382    | 0.20        | 1         |
| 81       | .     | 96  | HIS  | H    | 8.497      | 0.02        | 1         |
| 82       | .     | 96  | HIS  | HA   | 4.710      | 0.02        | 1         |
| 83       | .     | 96  | HIS  | HB2  | 3.131      | 0.02        | 2         |
| 84       | .     | 96  | HIS  | HB3  | 3.131      | 0.02        | 2         |
| 85       | .     | 96  | HIS  | HD2  | 7.133      | 0.02        | 1         |
| 86       | .     | 96  | HIS  | CA   | 55.332     | 0.20        | 1         |
| 87       | .     | 96  | HIS  | CB   | 29.114     | 0.20        | 1         |
| 88       | .     | 96  | HIS  | CD2  | 119.845    | 0.20        | 1         |
| 89       | .     | 96  | HIS  | N    | 120.663    | 0.20        | 1         |
| 90       | .     | 97  | SER  | H    | 8.255      | 0.02        | 1         |
| 91       | .     | 97  | SER  | HA   | 4.375      | 0.02        | 1         |
| 92       | .     | 97  | SER  | HB2  | 3.805      | 0.02        | 2         |
| 93       | .     | 97  | SER  | HB3  | 3.756      | 0.02        | 2         |
| 94       | .     | 97  | SER  | CA   | 58.520     | 0.20        | 1         |
| 95       | .     | 97  | SER  | CB   | 63.724     | 0.20        | 1         |
| 96       | .     | 97  | SER  | N    | 116.790    | 0.20        | 1         |
| 97       | .     | 98  | GLN  | H    | 8.452      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 98       | .     | 98  | GLN  | HA   | 4.275      | 0.02        | 1         |
| 99       | .     | 98  | GLN  | HB2  | 1.952      | 0.02        | 2         |
| 100      | .     | 98  | GLN  | HB3  | 1.859      | 0.02        | 2         |
| 101      | .     | 98  | GLN  | HG2  | 2.149      | 0.02        | 2         |
| 102      | .     | 98  | GLN  | HG3  | 2.149      | 0.02        | 2         |
| 103      | .     | 98  | GLN  | HE21 | 7.215      | 0.02        | 2         |
| 104      | .     | 98  | GLN  | HE22 | 7.323      | 0.02        | 2         |
| 105      | .     | 98  | GLN  | CA   | 56.116     | 0.20        | 1         |
| 106      | .     | 98  | GLN  | CB   | 29.194     | 0.20        | 1         |
| 107      | .     | 98  | GLN  | CG   | 33.539     | 0.20        | 1         |
| 108      | .     | 98  | GLN  | N    | 121.973    | 0.20        | 1         |
| 109      | .     | 98  | GLN  | NE2  | 110.654    | 0.20        | 1         |
| 110      | .     | 99  | TRP  | H    | 8.066      | 0.02        | 1         |
| 111      | .     | 99  | TRP  | HA   | 4.671      | 0.02        | 1         |
| 112      | .     | 99  | TRP  | HB2  | 3.295      | 0.02        | 2         |
| 113      | .     | 99  | TRP  | HB3  | 3.191      | 0.02        | 2         |
| 114      | .     | 99  | TRP  | HD1  | 7.228      | 0.02        | 1         |
| 115      | .     | 99  | TRP  | HE1  | 10.096     | 0.02        | 1         |
| 116      | .     | 99  | TRP  | HE3  | 7.597      | 0.02        | 1         |
| 117      | .     | 99  | TRP  | HZ2  | 7.449      | 0.02        | 1         |
| 118      | .     | 99  | TRP  | HZ3  | 7.114      | 0.02        | 1         |
| 119      | .     | 99  | TRP  | HH2  | 7.201      | 0.02        | 1         |
| 120      | .     | 99  | TRP  | CA   | 57.154     | 0.20        | 1         |
| 121      | .     | 99  | TRP  | CB   | 29.465     | 0.20        | 1         |
| 122      | .     | 99  | TRP  | CD1  | 126.917    | 0.20        | 1         |
| 123      | .     | 99  | TRP  | CE3  | 120.877    | 0.20        | 1         |
| 124      | .     | 99  | TRP  | CZ2  | 114.544    | 0.20        | 1         |
| 125      | .     | 99  | TRP  | CZ3  | 122.017    | 0.20        | 1         |
| 126      | .     | 99  | TRP  | CH2  | 124.650    | 0.20        | 1         |
| 127      | .     | 99  | TRP  | N    | 121.479    | 0.20        | 1         |
| 128      | .     | 99  | TRP  | NE1  | 129.287    | 0.20        | 1         |
| 129      | .     | 100 | ASN  | H    | 8.080      | 0.02        | 1         |
| 130      | .     | 100 | ASN  | HA   | 4.604      | 0.02        | 1         |
| 131      | .     | 100 | ASN  | HB2  | 2.554      | 0.02        | 2         |
| 132      | .     | 100 | ASN  | HB3  | 2.534      | 0.02        | 2         |
| 133      | .     | 100 | ASN  | HD21 | 6.812      | 0.02        | 2         |
| 134      | .     | 100 | ASN  | HD22 | 7.438      | 0.02        | 2         |
| 135      | .     | 100 | ASN  | CA   | 52.773     | 0.20        | 1         |
| 136      | .     | 100 | ASN  | CB   | 38.807     | 0.20        | 1         |
| 137      | .     | 100 | ASN  | N    | 120.389    | 0.20        | 1         |
| 138      | .     | 100 | ASN  | ND2  | 112.422    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 139      | .     | 101 | LYS  | H    | 7.958      | 0.02        | 1         |
| 140      | .     | 101 | LYS  | HA   | 4.449      | 0.02        | 1         |
| 141      | .     | 101 | LYS  | HB2  | 1.762      | 0.02        | 2         |
| 142      | .     | 101 | LYS  | HB3  | 1.633      | 0.02        | 2         |
| 143      | .     | 101 | LYS  | HG2  | 1.364      | 0.02        | 2         |
| 144      | .     | 101 | LYS  | HG3  | 1.364      | 0.02        | 2         |
| 145      | .     | 101 | LYS  | HD2  | 1.692      | 0.02        | 2         |
| 146      | .     | 101 | LYS  | HD3  | 1.661      | 0.02        | 2         |
| 147      | .     | 101 | LYS  | HE2  | 2.967      | 0.02        | 2         |
| 148      | .     | 101 | LYS  | HE3  | 2.967      | 0.02        | 2         |
| 149      | .     | 101 | LYS  | CA   | 54.217     | 0.20        | 1         |
| 150      | .     | 101 | LYS  | CB   | 32.558     | 0.20        | 1         |
| 151      | .     | 101 | LYS  | CG   | 24.636     | 0.20        | 1         |
| 152      | .     | 101 | LYS  | CD   | 29.105     | 0.20        | 1         |
| 153      | .     | 101 | LYS  | CE   | 41.943     | 0.20        | 1         |
| 154      | .     | 101 | LYS  | N    | 122.513    | 0.20        | 1         |
| 155      | .     | 102 | PRO  | HA   | 4.430      | 0.02        | 1         |
| 156      | .     | 102 | PRO  | HB2  | 2.284      | 0.02        | 2         |
| 157      | .     | 102 | PRO  | HB3  | 1.897      | 0.02        | 2         |
| 158      | .     | 102 | PRO  | HG2  | 2.005      | 0.02        | 2         |
| 159      | .     | 102 | PRO  | HG3  | 2.005      | 0.02        | 2         |
| 160      | .     | 102 | PRO  | HD2  | 3.783      | 0.02        | 2         |
| 161      | .     | 102 | PRO  | HD3  | 3.621      | 0.02        | 2         |
| 162      | .     | 102 | PRO  | CA   | 63.190     | 0.20        | 1         |
| 163      | .     | 102 | PRO  | CB   | 32.222     | 0.20        | 1         |
| 164      | .     | 102 | PRO  | CG   | 27.379     | 0.20        | 1         |
| 165      | .     | 102 | PRO  | CD   | 50.754     | 0.20        | 1         |
| 166      | .     | 103 | SER  | H    | 8.401      | 0.02        | 1         |
| 167      | .     | 103 | SER  | HA   | 4.428      | 0.02        | 1         |
| 168      | .     | 103 | SER  | HB2  | 3.831      | 0.02        | 2         |
| 169      | .     | 103 | SER  | HB3  | 3.831      | 0.02        | 2         |
| 170      | .     | 103 | SER  | CA   | 58.099     | 0.20        | 1         |
| 171      | .     | 103 | SER  | CB   | 63.967     | 0.20        | 1         |
| 172      | .     | 103 | SER  | N    | 116.774    | 0.20        | 1         |
| 173      | .     | 104 | LYS  | H    | 8.295      | 0.02        | 1         |
| 174      | .     | 104 | LYS  | HA   | 4.619      | 0.02        | 1         |
| 175      | .     | 104 | LYS  | HB2  | 1.758      | 0.02        | 2         |
| 176      | .     | 104 | LYS  | HB3  | 1.722      | 0.02        | 2         |
| 177      | .     | 104 | LYS  | HG2  | 1.460      | 0.02        | 2         |
| 178      | .     | 104 | LYS  | HG3  | 1.442      | 0.02        | 2         |
| 179      | .     | 104 | LYS  | HD2  | 1.687      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 180      | .     | 104 | LYS  | HD3  | 1.687      | 0.02        | 2         |
| 181      | .     | 104 | LYS  | HE2  | 3.003      | 0.02        | 2         |
| 182      | .     | 104 | LYS  | HE3  | 2.996      | 0.02        | 2         |
| 183      | .     | 104 | LYS  | CA   | 54.231     | 0.20        | 1         |
| 184      | .     | 104 | LYS  | CB   | 32.941     | 0.20        | 1         |
| 185      | .     | 104 | LYS  | CG   | 24.944     | 0.20        | 1         |
| 186      | .     | 104 | LYS  | CD   | 29.157     | 0.20        | 1         |
| 187      | .     | 104 | LYS  | CE   | 41.983     | 0.20        | 1         |
| 188      | .     | 104 | LYS  | N    | 124.057    | 0.20        | 1         |
| 189      | .     | 105 | PRO  | HA   | 4.408      | 0.02        | 1         |
| 190      | .     | 105 | PRO  | HB2  | 2.284      | 0.02        | 2         |
| 191      | .     | 105 | PRO  | HB3  | 1.894      | 0.02        | 2         |
| 192      | .     | 105 | PRO  | HG2  | 2.016      | 0.02        | 2         |
| 193      | .     | 105 | PRO  | HG3  | 2.016      | 0.02        | 2         |
| 194      | .     | 105 | PRO  | HD2  | 3.620      | 0.02        | 2         |
| 195      | .     | 105 | PRO  | HD3  | 3.865      | 0.02        | 2         |
| 196      | .     | 105 | PRO  | CA   | 63.111     | 0.20        | 1         |
| 197      | .     | 105 | PRO  | CB   | 32.256     | 0.20        | 1         |
| 198      | .     | 105 | PRO  | CG   | 27.390     | 0.20        | 1         |
| 199      | .     | 105 | PRO  | CD   | 50.856     | 0.20        | 1         |
| 200      | .     | 106 | LYS  | H    | 8.500      | 0.02        | 1         |
| 201      | .     | 106 | LYS  | HA   | 4.339      | 0.02        | 1         |
| 202      | .     | 106 | LYS  | HB2  | 1.744      | 0.02        | 2         |
| 203      | .     | 106 | LYS  | HB3  | 1.861      | 0.02        | 2         |
| 204      | .     | 106 | LYS  | HG2  | 1.502      | 0.02        | 2         |
| 205      | .     | 106 | LYS  | HG3  | 1.450      | 0.02        | 2         |
| 206      | .     | 106 | LYS  | HD2  | 1.692      | 0.02        | 2         |
| 207      | .     | 106 | LYS  | HD3  | 1.662      | 0.02        | 2         |
| 208      | .     | 106 | LYS  | HE2  | 2.967      | 0.02        | 2         |
| 209      | .     | 106 | LYS  | HE3  | 2.967      | 0.02        | 2         |
| 210      | .     | 106 | LYS  | CA   | 56.280     | 0.20        | 1         |
| 211      | .     | 106 | LYS  | CB   | 33.024     | 0.20        | 1         |
| 212      | .     | 106 | LYS  | CG   | 24.855     | 0.20        | 1         |
| 213      | .     | 106 | LYS  | CD   | 29.116     | 0.20        | 1         |
| 214      | .     | 106 | LYS  | CE   | 42.027     | 0.20        | 1         |
| 215      | .     | 106 | LYS  | N    | 122.002    | 0.20        | 1         |
| 216      | .     | 107 | THR  | H    | 8.118      | 0.02        | 1         |
| 217      | .     | 107 | THR  | HA   | 4.324      | 0.02        | 1         |
| 218      | .     | 107 | THR  | HB   | 4.167      | 0.02        | 1         |
| 219      | .     | 107 | THR  | HG2  | 1.178      | 0.02        | 1         |
| 220      | .     | 107 | THR  | HG2  | 1.178      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 221      | .     | 107 | THR  | HG2  | 1.178      | 0.02        | 1         |
| 222      | .     | 107 | THR  | CA   | 61.636     | 0.20        | 1         |
| 223      | .     | 107 | THR  | CB   | 69.771     | 0.20        | 1         |
| 224      | .     | 107 | THR  | CG2  | 21.583     | 0.20        | 1         |
| 225      | .     | 107 | THR  | N    | 115.105    | 0.20        | 1         |
| 226      | .     | 108 | ASN  | H    | 8.516      | 0.02        | 1         |
| 227      | .     | 108 | ASN  | HA   | 4.712      | 0.02        | 1         |
| 228      | .     | 108 | ASN  | HB2  | 2.835      | 0.02        | 2         |
| 229      | .     | 108 | ASN  | HB3  | 2.760      | 0.02        | 2         |
| 230      | .     | 108 | ASN  | HD21 | 7.577      | 0.02        | 2         |
| 231      | .     | 108 | ASN  | HD22 | 6.879      | 0.02        | 2         |
| 232      | .     | 108 | ASN  | CA   | 53.145     | 0.20        | 1         |
| 233      | .     | 108 | ASN  | CB   | 38.771     | 0.20        | 1         |
| 234      | .     | 108 | ASN  | N    | 121.228    | 0.20        | 1         |
| 235      | .     | 108 | ASN  | ND2  | 112.580    | 0.20        | 1         |
| 236      | .     | 109 | MET  | H    | 8.324      | 0.02        | 1         |
| 237      | .     | 109 | MET  | HA   | 4.435      | 0.02        | 1         |
| 238      | .     | 109 | MET  | HB2  | 2.003      | 0.02        | 2         |
| 239      | .     | 109 | MET  | HB3  | 1.965      | 0.02        | 2         |
| 240      | .     | 109 | MET  | HG2  | 2.563      | 0.02        | 2         |
| 241      | .     | 109 | MET  | HG3  | 2.490      | 0.02        | 2         |
| 242      | .     | 109 | MET  | HE   | 2.073      | 0.02        | 1         |
| 243      | .     | 109 | MET  | HE   | 2.073      | 0.02        | 1         |
| 244      | .     | 109 | MET  | HE   | 2.073      | 0.02        | 1         |
| 245      | .     | 109 | MET  | CA   | 55.565     | 0.20        | 1         |
| 246      | .     | 109 | MET  | CB   | 32.811     | 0.20        | 1         |
| 247      | .     | 109 | MET  | CG   | 32.037     | 0.20        | 1         |
| 248      | .     | 109 | MET  | CE   | 16.988     | 0.20        | 1         |
| 249      | .     | 109 | MET  | N    | 121.188    | 0.20        | 1         |
| 250      | .     | 110 | LYS  | H    | 8.284      | 0.02        | 1         |
| 251      | .     | 110 | LYS  | HA   | 4.234      | 0.02        | 1         |
| 252      | .     | 110 | LYS  | HB2  | 1.723      | 0.02        | 2         |
| 253      | .     | 110 | LYS  | HB3  | 1.753      | 0.02        | 2         |
| 254      | .     | 110 | LYS  | HG2  | 1.406      | 0.02        | 2         |
| 255      | .     | 110 | LYS  | HG3  | 1.342      | 0.02        | 2         |
| 256      | .     | 110 | LYS  | HD2  | 1.692      | 0.02        | 2         |
| 257      | .     | 110 | LYS  | HD3  | 1.662      | 0.02        | 2         |
| 258      | .     | 110 | LYS  | HE2  | 2.973      | 0.02        | 2         |
| 259      | .     | 110 | LYS  | HE3  | 2.960      | 0.02        | 2         |
| 260      | .     | 110 | LYS  | CA   | 56.468     | 0.20        | 1         |
| 261      | .     | 110 | LYS  | CB   | 33.001     | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 262      | .     | 110 | LYS  | CG   | 24.903     | 0.20        | 1         |
| 263      | .     | 110 | LYS  | CD   | 29.048     | 0.20        | 1         |
| 264      | .     | 110 | LYS  | CE   | 42.063     | 0.20        | 1         |
| 265      | .     | 110 | LYS  | N    | 122.137    | 0.20        | 1         |
| 266      | .     | 111 | HIS  | H    | 8.427      | 0.02        | 1         |
| 267      | .     | 111 | HIS  | HA   | 4.658      | 0.02        | 1         |
| 268      | .     | 111 | HIS  | HB2  | 3.208      | 0.02        | 2         |
| 269      | .     | 111 | HIS  | HB3  | 3.190      | 0.02        | 2         |
| 270      | .     | 111 | HIS  | HD2  | 7.133      | 0.02        | 1         |
| 271      | .     | 111 | HIS  | CA   | 55.368     | 0.20        | 1         |
| 272      | .     | 111 | HIS  | CB   | 29.515     | 0.20        | 1         |
| 273      | .     | 111 | HIS  | CD2  | 119.845    | 0.20        | 1         |
| 274      | .     | 111 | HIS  | N    | 119.887    | 0.20        | 1         |
| 275      | .     | 112 | MET  | H    | 8.347      | 0.02        | 1         |
| 276      | .     | 112 | MET  | HA   | 4.464      | 0.02        | 1         |
| 277      | .     | 112 | MET  | HB2  | 2.059      | 0.02        | 2         |
| 278      | .     | 112 | MET  | HB3  | 1.957      | 0.02        | 2         |
| 279      | .     | 112 | MET  | HG2  | 2.565      | 0.02        | 2         |
| 280      | .     | 112 | MET  | HG3  | 2.490      | 0.02        | 2         |
| 281      | .     | 112 | MET  | HE   | 2.073      | 0.02        | 1         |
| 282      | .     | 112 | MET  | HE   | 2.073      | 0.02        | 1         |
| 283      | .     | 112 | MET  | HE   | 2.073      | 0.02        | 1         |
| 284      | .     | 112 | MET  | CA   | 55.165     | 0.20        | 1         |
| 285      | .     | 112 | MET  | CB   | 33.002     | 0.20        | 1         |
| 286      | .     | 112 | MET  | CG   | 32.060     | 0.20        | 1         |
| 287      | .     | 112 | MET  | CE   | 17.048     | 0.20        | 1         |
| 288      | .     | 112 | MET  | N    | 122.440    | 0.20        | 1         |
| 289      | .     | 113 | ALA  | H    | 8.382      | 0.02        | 1         |
| 290      | .     | 113 | ALA  | HA   | 4.295      | 0.02        | 1         |
| 291      | .     | 113 | ALA  | HB   | 1.381      | 0.02        | 1         |
| 292      | .     | 113 | ALA  | HB   | 1.381      | 0.02        | 1         |
| 293      | .     | 113 | ALA  | HB   | 1.381      | 0.02        | 1         |
| 294      | .     | 113 | ALA  | CA   | 52.682     | 0.20        | 1         |
| 295      | .     | 113 | ALA  | CB   | 19.292     | 0.20        | 1         |
| 296      | .     | 113 | ALA  | N    | 125.614    | 0.20        | 1         |
| 297      | .     | 114 | GLY  | H    | 8.378      | 0.02        | 1         |
| 298      | .     | 114 | GLY  | HA2  | 3.936      | 0.02        | 2         |
| 299      | .     | 114 | GLY  | HA3  | 3.924      | 0.02        | 2         |
| 300      | .     | 114 | GLY  | CA   | 45.256     | 0.20        | 1         |
| 301      | .     | 114 | GLY  | N    | 108.485    | 0.20        | 1         |
| 302      | .     | 115 | ALA  | H    | 8.123      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 303      | .     | 115 | ALA  | HA   | 4.293      | 0.02        | 1         |
| 304      | .     | 115 | ALA  | HB   | 1.381      | 0.02        | 1         |
| 305      | .     | 115 | ALA  | HB   | 1.381      | 0.02        | 1         |
| 306      | .     | 115 | ALA  | HB   | 1.381      | 0.02        | 1         |
| 307      | .     | 115 | ALA  | CA   | 52.600     | 0.20        | 1         |
| 308      | .     | 115 | ALA  | CB   | 19.356     | 0.20        | 1         |
| 309      | .     | 115 | ALA  | N    | 123.808    | 0.20        | 1         |
| 310      | .     | 116 | ALA  | H    | 8.174      | 0.02        | 1         |
| 311      | .     | 116 | ALA  | HA   | 4.295      | 0.02        | 1         |
| 312      | .     | 116 | ALA  | HB   | 1.384      | 0.02        | 1         |
| 313      | .     | 116 | ALA  | HB   | 1.384      | 0.02        | 1         |
| 314      | .     | 116 | ALA  | HB   | 1.384      | 0.02        | 1         |
| 315      | .     | 116 | ALA  | CA   | 52.532     | 0.20        | 1         |
| 316      | .     | 116 | ALA  | CB   | 19.259     | 0.20        | 1         |
| 317      | .     | 116 | ALA  | N    | 123.151    | 0.20        | 1         |
| 318      | .     | 117 | ALA  | H    | 8.207      | 0.02        | 1         |
| 319      | .     | 117 | ALA  | HA   | 4.285      | 0.02        | 1         |
| 320      | .     | 117 | ALA  | HB   | 1.384      | 0.02        | 1         |
| 321      | .     | 117 | ALA  | HB   | 1.384      | 0.02        | 1         |
| 322      | .     | 117 | ALA  | HB   | 1.384      | 0.02        | 1         |
| 323      | .     | 117 | ALA  | CA   | 52.559     | 0.20        | 1         |
| 324      | .     | 117 | ALA  | CB   | 19.284     | 0.20        | 1         |
| 325      | .     | 117 | ALA  | N    | 123.151    | 0.20        | 1         |
| 326      | .     | 118 | ALA  | H    | 8.260      | 0.02        | 1         |
| 327      | .     | 118 | ALA  | HA   | 4.297      | 0.02        | 1         |
| 328      | .     | 118 | ALA  | HB   | 1.374      | 0.02        | 1         |
| 329      | .     | 118 | ALA  | HB   | 1.374      | 0.02        | 1         |
| 330      | .     | 118 | ALA  | HB   | 1.374      | 0.02        | 1         |
| 331      | .     | 118 | ALA  | CA   | 52.626     | 0.20        | 1         |
| 332      | .     | 118 | ALA  | CB   | 19.230     | 0.20        | 1         |
| 333      | .     | 118 | ALA  | N    | 123.074    | 0.20        | 1         |
| 334      | .     | 119 | GLY  | H    | 8.248      | 0.02        | 1         |
| 335      | .     | 119 | GLY  | HA2  | 3.936      | 0.02        | 2         |
| 336      | .     | 119 | GLY  | HA3  | 3.924      | 0.02        | 2         |
| 337      | .     | 119 | GLY  | CA   | 45.282     | 0.20        | 1         |
| 338      | .     | 119 | GLY  | N    | 107.856    | 0.20        | 1         |
| 339      | .     | 120 | ALA  | H    | 8.049      | 0.02        | 1         |
| 340      | .     | 120 | ALA  | HA   | 4.373      | 0.02        | 1         |
| 341      | .     | 120 | ALA  | HB   | 1.378      | 0.02        | 1         |
| 342      | .     | 120 | ALA  | HB   | 1.378      | 0.02        | 1         |
| 343      | .     | 120 | ALA  | HB   | 1.378      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 344      | .     | 120 | ALA  | CA   | 52.274     | 0.20        | 1         |
| 345      | .     | 120 | ALA  | CB   | 19.375     | 0.20        | 1         |
| 346      | .     | 120 | ALA  | N    | 123.476    | 0.20        | 1         |
| 347      | .     | 121 | VAL  | H    | 8.103      | 0.02        | 1         |
| 348      | .     | 121 | VAL  | HA   | 4.137      | 0.02        | 1         |
| 349      | .     | 121 | VAL  | HB   | 2.003      | 0.02        | 1         |
| 350      | .     | 121 | VAL  | HG1  | 0.893      | 0.02        | 2         |
| 351      | .     | 121 | VAL  | HG1  | 0.893      | 0.02        | 2         |
| 352      | .     | 121 | VAL  | HG1  | 0.893      | 0.02        | 2         |
| 353      | .     | 121 | VAL  | HG2  | 0.848      | 0.02        | 2         |
| 354      | .     | 121 | VAL  | HG2  | 0.848      | 0.02        | 2         |
| 355      | .     | 121 | VAL  | HG2  | 0.848      | 0.02        | 2         |
| 356      | .     | 121 | VAL  | CA   | 62.209     | 0.20        | 1         |
| 357      | .     | 121 | VAL  | CB   | 32.802     | 0.20        | 1         |
| 358      | .     | 121 | VAL  | CG1  | 20.779     | 0.20        | 2         |
| 359      | .     | 121 | VAL  | CG2  | 21.278     | 0.20        | 2         |
| 360      | .     | 121 | VAL  | N    | 119.560    | 0.20        | 1         |
| 361      | .     | 122 | VAL  | H    | 8.246      | 0.02        | 1         |
| 362      | .     | 122 | VAL  | HA   | 4.087      | 0.02        | 1         |
| 363      | .     | 122 | VAL  | HB   | 1.984      | 0.02        | 1         |
| 364      | .     | 122 | VAL  | HG1  | 0.893      | 0.02        | 2         |
| 365      | .     | 122 | VAL  | HG1  | 0.893      | 0.02        | 2         |
| 366      | .     | 122 | VAL  | HG1  | 0.893      | 0.02        | 2         |
| 367      | .     | 122 | VAL  | HG2  | 0.848      | 0.02        | 2         |
| 368      | .     | 122 | VAL  | HG2  | 0.848      | 0.02        | 2         |
| 369      | .     | 122 | VAL  | HG2  | 0.848      | 0.02        | 2         |
| 370      | .     | 122 | VAL  | CA   | 62.455     | 0.20        | 1         |
| 371      | .     | 122 | VAL  | CB   | 32.753     | 0.20        | 1         |
| 372      | .     | 122 | VAL  | CG1  | 20.800     | 0.20        | 2         |
| 373      | .     | 122 | VAL  | CG2  | 21.301     | 0.20        | 2         |
| 374      | .     | 122 | VAL  | N    | 124.610    | 0.20        | 1         |
| 375      | .     | 123 | GLY  | H    | 8.554      | 0.02        | 1         |
| 376      | .     | 123 | GLY  | HA2  | 3.931      | 0.02        | 2         |
| 377      | .     | 123 | GLY  | HA3  | 3.931      | 0.02        | 2         |
| 378      | .     | 123 | GLY  | CA   | 45.291     | 0.20        | 1         |
| 379      | .     | 123 | GLY  | N    | 113.357    | 0.20        | 1         |
| 380      | .     | 124 | GLY  | H    | 8.249      | 0.02        | 1         |
| 381      | .     | 124 | GLY  | HA2  | 3.936      | 0.02        | 2         |
| 382      | .     | 124 | GLY  | HA3  | 3.936      | 0.02        | 2         |
| 383      | .     | 124 | GLY  | CA   | 45.305     | 0.20        | 1         |
| 384      | .     | 124 | GLY  | N    | 108.401    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 385      | .     | 125 | LEU  | H    | 8.182      | 0.02        | 1         |
| 386      | .     | 125 | LEU  | HA   | 4.376      | 0.02        | 1         |
| 387      | .     | 125 | LEU  | HB2  | 1.551      | 0.02        | 2         |
| 388      | .     | 125 | LEU  | HB3  | 1.617      | 0.02        | 2         |
| 389      | .     | 125 | LEU  | HG   | 1.510      | 0.02        | 1         |
| 390      | .     | 125 | LEU  | HD1  | 0.706      | 0.02        | 2         |
| 391      | .     | 125 | LEU  | HD1  | 0.706      | 0.02        | 2         |
| 392      | .     | 125 | LEU  | HD1  | 0.706      | 0.02        | 2         |
| 393      | .     | 125 | LEU  | HD2  | 0.605      | 0.02        | 2         |
| 394      | .     | 125 | LEU  | HD2  | 0.605      | 0.02        | 2         |
| 395      | .     | 125 | LEU  | HD2  | 0.605      | 0.02        | 2         |
| 396      | .     | 125 | LEU  | CA   | 54.875     | 0.20        | 1         |
| 397      | .     | 125 | LEU  | CB   | 42.587     | 0.20        | 1         |
| 398      | .     | 125 | LEU  | CG   | 27.009     | 0.20        | 1         |
| 399      | .     | 125 | LEU  | CD1  | 24.794     | 0.20        | 2         |
| 400      | .     | 125 | LEU  | CD2  | 23.594     | 0.20        | 2         |
| 401      | .     | 125 | LEU  | N    | 121.788    | 0.20        | 1         |
| 402      | .     | 126 | GLY  | H    | 8.488      | 0.02        | 1         |
| 403      | .     | 126 | GLY  | HA2  | 3.927      | 0.02        | 2         |
| 404      | .     | 126 | GLY  | HA3  | 3.839      | 0.02        | 2         |
| 405      | .     | 126 | GLY  | CA   | 46.047     | 0.20        | 1         |
| 406      | .     | 126 | GLY  | N    | 109.719    | 0.20        | 1         |
| 407      | .     | 127 | GLY  | H    | 8.298      | 0.02        | 1         |
| 408      | .     | 127 | GLY  | HA2  | 3.736      | 0.02        | 2         |
| 409      | .     | 127 | GLY  | HA3  | 3.931      | 0.02        | 2         |
| 410      | .     | 127 | GLY  | CA   | 45.112     | 0.20        | 1         |
| 411      | .     | 127 | GLY  | N    | 108.892    | 0.20        | 1         |
| 412      | .     | 128 | TYR  | H    | 7.691      | 0.02        | 1         |
| 413      | .     | 128 | TYR  | HA   | 4.492      | 0.02        | 1         |
| 414      | .     | 128 | TYR  | HB2  | 2.844      | 0.02        | 2         |
| 415      | .     | 128 | TYR  | HB3  | 2.951      | 0.02        | 2         |
| 416      | .     | 128 | TYR  | HD1  | 6.813      | 0.02        | 3         |
| 417      | .     | 128 | TYR  | HD2  | 6.813      | 0.02        | 3         |
| 418      | .     | 128 | TYR  | HE1  | 6.658      | 0.02        | 3         |
| 419      | .     | 128 | TYR  | HE2  | 6.658      | 0.02        | 3         |
| 420      | .     | 128 | TYR  | CA   | 58.264     | 0.20        | 1         |
| 421      | .     | 128 | TYR  | CB   | 40.430     | 0.20        | 1         |
| 422      | .     | 128 | TYR  | CD1  | 132.839    | 0.20        | 3         |
| 423      | .     | 128 | TYR  | CD2  | 132.839    | 0.20        | 3         |
| 424      | .     | 128 | TYR  | CE1  | 118.066    | 0.20        | 3         |
| 425      | .     | 128 | TYR  | CE2  | 118.066    | 0.20        | 3         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 426      | .     | 128 | TYR  | N    | 117.459    | 0.20        | 1         |
| 427      | .     | 129 | MET  | H    | 8.977      | 0.02        | 1         |
| 428      | .     | 129 | MET  | HA   | 4.549      | 0.02        | 1         |
| 429      | .     | 129 | MET  | HB2  | 1.549      | 0.02        | 2         |
| 430      | .     | 129 | MET  | HB3  | 0.905      | 0.02        | 2         |
| 431      | .     | 129 | MET  | HG2  | 2.286      | 0.02        | 2         |
| 432      | .     | 129 | MET  | HG3  | 2.211      | 0.02        | 2         |
| 433      | .     | 129 | MET  | HE   | 1.995      | 0.02        | 1         |
| 434      | .     | 129 | MET  | HE   | 1.995      | 0.02        | 1         |
| 435      | .     | 129 | MET  | HE   | 1.995      | 0.02        | 1         |
| 436      | .     | 129 | MET  | CA   | 53.664     | 0.20        | 1         |
| 437      | .     | 129 | MET  | CB   | 34.752     | 0.20        | 1         |
| 438      | .     | 129 | MET  | CG   | 32.305     | 0.20        | 1         |
| 439      | .     | 129 | MET  | CE   | 17.266     | 0.20        | 1         |
| 440      | .     | 129 | MET  | N    | 120.735    | 0.20        | 1         |
| 441      | .     | 130 | LEU  | H    | 8.050      | 0.02        | 1         |
| 442      | .     | 130 | LEU  | HA   | 4.460      | 0.02        | 1         |
| 443      | .     | 130 | LEU  | HB2  | 1.606      | 0.02        | 2         |
| 444      | .     | 130 | LEU  | HB3  | 0.952      | 0.02        | 2         |
| 445      | .     | 130 | LEU  | HG   | 1.371      | 0.02        | 1         |
| 446      | .     | 130 | LEU  | HD1  | -0.032     | 0.02        | 2         |
| 447      | .     | 130 | LEU  | HD1  | -0.032     | 0.02        | 2         |
| 448      | .     | 130 | LEU  | HD1  | -0.032     | 0.02        | 2         |
| 449      | .     | 130 | LEU  | HD2  | 0.617      | 0.02        | 2         |
| 450      | .     | 130 | LEU  | HD2  | 0.617      | 0.02        | 2         |
| 451      | .     | 130 | LEU  | HD2  | 0.617      | 0.02        | 2         |
| 452      | .     | 130 | LEU  | CA   | 53.376     | 0.20        | 1         |
| 453      | .     | 130 | LEU  | CB   | 43.635     | 0.20        | 1         |
| 454      | .     | 130 | LEU  | CG   | 26.033     | 0.20        | 1         |
| 455      | .     | 130 | LEU  | CD1  | 21.697     | 0.20        | 2         |
| 456      | .     | 130 | LEU  | CD2  | 25.861     | 0.20        | 2         |
| 457      | .     | 130 | LEU  | N    | 121.372    | 0.20        | 1         |
| 458      | .     | 131 | GLY  | H    | 9.339      | 0.02        | 1         |
| 459      | .     | 131 | GLY  | HA2  | 4.420      | 0.02        | 2         |
| 460      | .     | 131 | GLY  | HA3  | 3.986      | 0.02        | 2         |
| 461      | .     | 131 | GLY  | CA   | 44.766     | 0.20        | 1         |
| 462      | .     | 131 | GLY  | N    | 115.005    | 0.20        | 1         |
| 463      | .     | 132 | SER  | H    | 8.360      | 0.02        | 1         |
| 464      | .     | 132 | SER  | HA   | 4.412      | 0.02        | 1         |
| 465      | .     | 132 | SER  | HB2  | 3.967      | 0.02        | 2         |
| 466      | .     | 132 | SER  | HB3  | 3.871      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 467      | .     | 132 | SER  | CA   | 58.446     | 0.20        | 1         |
| 468      | .     | 132 | SER  | CB   | 64.024     | 0.20        | 1         |
| 469      | .     | 132 | SER  | N    | 113.604    | 0.20        | 1         |
| 470      | .     | 133 | ALA  | H    | 8.754      | 0.02        | 1         |
| 471      | .     | 133 | ALA  | HA   | 4.427      | 0.02        | 1         |
| 472      | .     | 133 | ALA  | HB   | 1.275      | 0.02        | 1         |
| 473      | .     | 133 | ALA  | HB   | 1.275      | 0.02        | 1         |
| 474      | .     | 133 | ALA  | HB   | 1.275      | 0.02        | 1         |
| 475      | .     | 133 | ALA  | CA   | 53.016     | 0.20        | 1         |
| 476      | .     | 133 | ALA  | CB   | 18.576     | 0.20        | 1         |
| 477      | .     | 133 | ALA  | N    | 125.601    | 0.20        | 1         |
| 478      | .     | 134 | MET  | H    | 8.705      | 0.02        | 1         |
| 479      | .     | 134 | MET  | HA   | 4.741      | 0.02        | 1         |
| 480      | .     | 134 | MET  | HB2  | 1.996      | 0.02        | 2         |
| 481      | .     | 134 | MET  | HB3  | 2.033      | 0.02        | 2         |
| 482      | .     | 134 | MET  | HG2  | 2.460      | 0.02        | 2         |
| 483      | .     | 134 | MET  | HG3  | 2.417      | 0.02        | 2         |
| 484      | .     | 134 | MET  | HE   | 2.150      | 0.02        | 1         |
| 485      | .     | 134 | MET  | HE   | 2.150      | 0.02        | 1         |
| 486      | .     | 134 | MET  | HE   | 2.150      | 0.02        | 1         |
| 487      | .     | 134 | MET  | CA   | 53.939     | 0.20        | 1         |
| 488      | .     | 134 | MET  | CB   | 37.027     | 0.20        | 1         |
| 489      | .     | 134 | MET  | CG   | 31.080     | 0.20        | 1         |
| 490      | .     | 134 | MET  | CE   | 17.768     | 0.20        | 1         |
| 491      | .     | 134 | MET  | N    | 120.807    | 0.20        | 1         |
| 492      | .     | 135 | SER  | H    | 8.413      | 0.02        | 1         |
| 493      | .     | 135 | SER  | HA   | 4.334      | 0.02        | 1         |
| 494      | .     | 135 | SER  | HB2  | 3.816      | 0.02        | 2         |
| 495      | .     | 135 | SER  | HB3  | 3.733      | 0.02        | 2         |
| 496      | .     | 135 | SER  | CA   | 58.579     | 0.20        | 1         |
| 497      | .     | 135 | SER  | CB   | 63.064     | 0.20        | 1         |
| 498      | .     | 135 | SER  | N    | 116.232    | 0.20        | 1         |
| 499      | .     | 136 | ARG  | H    | 8.631      | 0.02        | 1         |
| 500      | .     | 136 | ARG  | HA   | 4.372      | 0.02        | 1         |
| 501      | .     | 136 | ARG  | HB2  | 1.692      | 0.02        | 2         |
| 502      | .     | 136 | ARG  | HB3  | 1.609      | 0.02        | 2         |
| 503      | .     | 136 | ARG  | HG2  | 1.929      | 0.02        | 2         |
| 504      | .     | 136 | ARG  | HG3  | 1.929      | 0.02        | 2         |
| 505      | .     | 136 | ARG  | HD2  | 3.158      | 0.02        | 2         |
| 506      | .     | 136 | ARG  | HD3  | 3.119      | 0.02        | 2         |
| 507      | .     | 136 | ARG  | CA   | 54.834     | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 508      | .     | 136 | ARG  | CB   | 29.182     | 0.20        | 1         |
| 509      | .     | 136 | ARG  | CG   | 28.711     | 0.20        | 1         |
| 510      | .     | 136 | ARG  | CD   | 43.501     | 0.20        | 1         |
| 511      | .     | 136 | ARG  | N    | 126.477    | 0.20        | 1         |
| 512      | .     | 137 | PRO  | HA   | 4.423      | 0.02        | 1         |
| 513      | .     | 137 | PRO  | HB2  | 1.731      | 0.02        | 2         |
| 514      | .     | 137 | PRO  | HB3  | 2.221      | 0.02        | 2         |
| 515      | .     | 137 | PRO  | HG2  | 1.983      | 0.02        | 2         |
| 516      | .     | 137 | PRO  | HG3  | 1.983      | 0.02        | 2         |
| 517      | .     | 137 | PRO  | HD2  | 3.930      | 0.02        | 2         |
| 518      | .     | 137 | PRO  | HD3  | 3.930      | 0.02        | 2         |
| 519      | .     | 137 | PRO  | CA   | 62.431     | 0.20        | 1         |
| 520      | .     | 137 | PRO  | CB   | 32.368     | 0.20        | 1         |
| 521      | .     | 137 | PRO  | CG   | 27.444     | 0.20        | 1         |
| 522      | .     | 137 | PRO  | CD   | 50.767     | 0.20        | 1         |
| 523      | .     | 138 | ILE  | H    | 8.623      | 0.02        | 1         |
| 524      | .     | 138 | ILE  | HA   | 4.153      | 0.02        | 1         |
| 525      | .     | 138 | ILE  | HB   | 1.904      | 0.02        | 1         |
| 526      | .     | 138 | ILE  | HG12 | 1.583      | 0.02        | 2         |
| 527      | .     | 138 | ILE  | HG13 | 1.369      | 0.02        | 2         |
| 528      | .     | 138 | ILE  | HG2  | 0.731      | 0.02        | 1         |
| 529      | .     | 138 | ILE  | HG2  | 0.731      | 0.02        | 1         |
| 530      | .     | 138 | ILE  | HG2  | 0.731      | 0.02        | 1         |
| 531      | .     | 138 | ILE  | HD1  | 0.889      | 0.02        | 1         |
| 532      | .     | 138 | ILE  | HD1  | 0.889      | 0.02        | 1         |
| 533      | .     | 138 | ILE  | HD1  | 0.889      | 0.02        | 1         |
| 534      | .     | 138 | ILE  | CA   | 60.790     | 0.20        | 1         |
| 535      | .     | 138 | ILE  | CB   | 36.385     | 0.20        | 1         |
| 536      | .     | 138 | ILE  | CG1  | 27.165     | 0.20        | 1         |
| 537      | .     | 138 | ILE  | CG2  | 17.482     | 0.20        | 1         |
| 538      | .     | 138 | ILE  | CD1  | 11.404     | 0.20        | 1         |
| 539      | .     | 138 | ILE  | N    | 122.606    | 0.20        | 1         |
| 540      | .     | 139 | ILE  | H    | 6.485      | 0.02        | 1         |
| 541      | .     | 139 | ILE  | HA   | 3.923      | 0.02        | 1         |
| 542      | .     | 139 | ILE  | HB   | 0.875      | 0.02        | 1         |
| 543      | .     | 139 | ILE  | HG12 | 0.892      | 0.02        | 2         |
| 544      | .     | 139 | ILE  | HG13 | 0.750      | 0.02        | 2         |
| 545      | .     | 139 | ILE  | HG2  | -0.039     | 0.02        | 1         |
| 546      | .     | 139 | ILE  | HG2  | -0.039     | 0.02        | 1         |
| 547      | .     | 139 | ILE  | HG2  | -0.039     | 0.02        | 1         |
| 548      | .     | 139 | ILE  | HD1  | 0.463      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 549      | .     | 139 | ILE  | HD1  | 0.463      | 0.02        | 1         |
| 550      | .     | 139 | ILE  | HD1  | 0.463      | 0.02        | 1         |
| 551      | .     | 139 | ILE  | CA   | 58.806     | 0.20        | 1         |
| 552      | .     | 139 | ILE  | CB   | 39.470     | 0.20        | 1         |
| 553      | .     | 139 | ILE  | CG1  | 26.708     | 0.20        | 1         |
| 554      | .     | 139 | ILE  | CG2  | 17.243     | 0.20        | 1         |
| 555      | .     | 139 | ILE  | CD1  | 12.703     | 0.20        | 1         |
| 556      | .     | 139 | ILE  | N    | 126.567    | 0.20        | 1         |
| 557      | .     | 140 | HIS  | H    | 8.223      | 0.02        | 1         |
| 558      | .     | 140 | HIS  | HA   | 4.919      | 0.02        | 1         |
| 559      | .     | 140 | HIS  | HB2  | 2.948      | 0.02        | 2         |
| 560      | .     | 140 | HIS  | HB3  | 3.296      | 0.02        | 2         |
| 561      | .     | 140 | HIS  | HD2  | 7.216      | 0.02        | 1         |
| 562      | .     | 140 | HIS  | HE1  | 8.473      | 0.02        | 1         |
| 563      | .     | 140 | HIS  | CA   | 54.157     | 0.20        | 1         |
| 564      | .     | 140 | HIS  | CB   | 29.486     | 0.20        | 1         |
| 565      | .     | 140 | HIS  | CD2  | 119.694    | 0.20        | 1         |
| 566      | .     | 140 | HIS  | CE1  | 136.389    | 0.20        | 1         |
| 567      | .     | 140 | HIS  | N    | 122.010    | 0.20        | 1         |
| 568      | .     | 141 | PHE  | H    | 10.126     | 0.02        | 1         |
| 569      | .     | 141 | PHE  | HA   | 4.360      | 0.02        | 1         |
| 570      | .     | 141 | PHE  | HB2  | 2.967      | 0.02        | 2         |
| 571      | .     | 141 | PHE  | HB3  | 2.742      | 0.02        | 2         |
| 572      | .     | 141 | PHE  | HD1  | 7.314      | 0.02        | 3         |
| 573      | .     | 141 | PHE  | HD2  | 7.313      | 0.02        | 3         |
| 574      | .     | 141 | PHE  | HE1  | 6.887      | 0.02        | 3         |
| 575      | .     | 141 | PHE  | HE2  | 6.887      | 0.02        | 3         |
| 576      | .     | 141 | PHE  | HZ   | 6.690      | 0.02        | 1         |
| 577      | .     | 141 | PHE  | CA   | 59.307     | 0.20        | 1         |
| 578      | .     | 141 | PHE  | CB   | 41.953     | 0.20        | 1         |
| 579      | .     | 141 | PHE  | CD1  | 132.091    | 0.20        | 3         |
| 580      | .     | 141 | PHE  | CD2  | 132.086    | 0.20        | 3         |
| 581      | .     | 141 | PHE  | CE1  | 131.359    | 0.20        | 3         |
| 582      | .     | 141 | PHE  | CE2  | 131.359    | 0.20        | 3         |
| 583      | .     | 141 | PHE  | CZ   | 129.296    | 0.20        | 1         |
| 584      | .     | 141 | PHE  | N    | 124.340    | 0.20        | 1         |
| 585      | .     | 142 | GLY  | H    | 8.989      | 0.02        | 1         |
| 586      | .     | 142 | GLY  | HA2  | 4.155      | 0.02        | 2         |
| 587      | .     | 142 | GLY  | HA3  | 3.834      | 0.02        | 2         |
| 588      | .     | 142 | GLY  | CA   | 45.689     | 0.20        | 1         |
| 589      | .     | 142 | GLY  | N    | 108.332    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 590      | .     | 143 | SER  | H    | 7.323      | 0.02        | 1         |
| 591      | .     | 143 | SER  | HA   | 4.808      | 0.02        | 1         |
| 592      | .     | 143 | SER  | HB2  | 4.116      | 0.02        | 2         |
| 593      | .     | 143 | SER  | HB3  | 3.924      | 0.02        | 2         |
| 594      | .     | 143 | SER  | CA   | 56.654     | 0.20        | 1         |
| 595      | .     | 143 | SER  | CB   | 66.028     | 0.20        | 1         |
| 596      | .     | 143 | SER  | N    | 111.807    | 0.20        | 1         |
| 597      | .     | 144 | ASP  | H    | 9.000      | 0.02        | 1         |
| 598      | .     | 144 | ASP  | HA   | 4.500      | 0.02        | 1         |
| 599      | .     | 144 | ASP  | HB2  | 2.741      | 0.02        | 2         |
| 600      | .     | 144 | ASP  | HB3  | 2.718      | 0.02        | 2         |
| 601      | .     | 144 | ASP  | CA   | 57.621     | 0.20        | 1         |
| 602      | .     | 144 | ASP  | CB   | 40.980     | 0.20        | 1         |
| 603      | .     | 144 | ASP  | N    | 124.251    | 0.20        | 1         |
| 604      | .     | 145 | TYR  | H    | 8.540      | 0.02        | 1         |
| 605      | .     | 145 | TYR  | HA   | 4.192      | 0.02        | 1         |
| 606      | .     | 145 | TYR  | HB2  | 2.847      | 0.02        | 2         |
| 607      | .     | 145 | TYR  | HB3  | 3.250      | 0.02        | 2         |
| 608      | .     | 145 | TYR  | HD1  | 7.051      | 0.02        | 3         |
| 609      | .     | 145 | TYR  | HD2  | 7.051      | 0.02        | 3         |
| 610      | .     | 145 | TYR  | HE1  | 6.756      | 0.02        | 3         |
| 611      | .     | 145 | TYR  | HE2  | 6.756      | 0.02        | 3         |
| 612      | .     | 145 | TYR  | CA   | 61.432     | 0.20        | 1         |
| 613      | .     | 145 | TYR  | CB   | 38.177     | 0.20        | 1         |
| 614      | .     | 145 | TYR  | CD1  | 133.336    | 0.20        | 3         |
| 615      | .     | 145 | TYR  | CD2  | 133.336    | 0.20        | 3         |
| 616      | .     | 145 | TYR  | CE1  | 118.407    | 0.20        | 3         |
| 617      | .     | 145 | TYR  | CE2  | 118.421    | 0.20        | 3         |
| 618      | .     | 145 | TYR  | N    | 118.980    | 0.20        | 1         |
| 619      | .     | 146 | GLU  | H    | 7.736      | 0.02        | 1         |
| 620      | .     | 146 | GLU  | HA   | 3.558      | 0.02        | 1         |
| 621      | .     | 146 | GLU  | HB2  | 1.891      | 0.02        | 2         |
| 622      | .     | 146 | GLU  | HB3  | 1.550      | 0.02        | 2         |
| 623      | .     | 146 | GLU  | HG2  | 1.898      | 0.02        | 2         |
| 624      | .     | 146 | GLU  | HG3  | 2.237      | 0.02        | 2         |
| 625      | .     | 146 | GLU  | CA   | 59.947     | 0.20        | 1         |
| 626      | .     | 146 | GLU  | CB   | 30.252     | 0.20        | 1         |
| 627      | .     | 146 | GLU  | CG   | 38.109     | 0.20        | 1         |
| 628      | .     | 146 | GLU  | N    | 119.203    | 0.20        | 1         |
| 629      | .     | 148 | ARG  | H    | 8.179      | 0.02        | 1         |
| 630      | .     | 148 | ARG  | HA   | 3.999      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 631      | .     | 148 | ARG  | HB2  | 1.893      | 0.02        | 2         |
| 632      | .     | 148 | ARG  | HB3  | 1.893      | 0.02        | 2         |
| 633      | .     | 148 | ARG  | HG2  | 1.738      | 0.02        | 2         |
| 634      | .     | 148 | ARG  | HG3  | 1.528      | 0.02        | 2         |
| 635      | .     | 148 | ARG  | HD2  | 3.219      | 0.02        | 2         |
| 636      | .     | 148 | ARG  | HD3  | 3.157      | 0.02        | 2         |
| 637      | .     | 148 | ARG  | CA   | 59.648     | 0.20        | 1         |
| 638      | .     | 148 | ARG  | CB   | 29.924     | 0.20        | 1         |
| 639      | .     | 148 | ARG  | CG   | 27.840     | 0.20        | 1         |
| 640      | .     | 148 | ARG  | CD   | 43.430     | 0.20        | 1         |
| 641      | .     | 148 | ARG  | N    | 120.241    | 0.20        | 1         |
| 642      | .     | 149 | TYR  | H    | 8.318      | 0.02        | 1         |
| 643      | .     | 149 | TYR  | HA   | 3.819      | 0.02        | 1         |
| 644      | .     | 149 | TYR  | HB2  | 2.557      | 0.02        | 2         |
| 645      | .     | 149 | TYR  | HB3  | 2.843      | 0.02        | 2         |
| 646      | .     | 149 | TYR  | HD1  | 6.898      | 0.02        | 3         |
| 647      | .     | 149 | TYR  | HD2  | 6.898      | 0.02        | 3         |
| 648      | .     | 149 | TYR  | HE1  | 6.854      | 0.02        | 3         |
| 649      | .     | 149 | TYR  | HE2  | 6.854      | 0.02        | 3         |
| 650      | .     | 149 | TYR  | CA   | 62.254     | 0.20        | 1         |
| 651      | .     | 149 | TYR  | CB   | 38.542     | 0.20        | 1         |
| 652      | .     | 149 | TYR  | CD1  | 133.017    | 0.20        | 3         |
| 653      | .     | 149 | TYR  | CD2  | 133.025    | 0.20        | 3         |
| 654      | .     | 149 | TYR  | CE1  | 118.060    | 0.20        | 3         |
| 655      | .     | 149 | TYR  | CE2  | 118.060    | 0.20        | 3         |
| 656      | .     | 149 | TYR  | N    | 121.174    | 0.20        | 1         |
| 657      | .     | 150 | TYR  | H    | 8.932      | 0.02        | 1         |
| 658      | .     | 150 | TYR  | HA   | 4.121      | 0.02        | 1         |
| 659      | .     | 150 | TYR  | HB2  | 3.162      | 0.02        | 2         |
| 660      | .     | 150 | TYR  | HB3  | 3.540      | 0.02        | 2         |
| 661      | .     | 150 | TYR  | HD1  | 7.526      | 0.02        | 3         |
| 662      | .     | 150 | TYR  | HD2  | 7.526      | 0.02        | 3         |
| 663      | .     | 150 | TYR  | HE1  | 7.011      | 0.02        | 3         |
| 664      | .     | 150 | TYR  | HE2  | 7.011      | 0.02        | 3         |
| 665      | .     | 150 | TYR  | CA   | 63.031     | 0.20        | 1         |
| 666      | .     | 150 | TYR  | CB   | 38.243     | 0.20        | 1         |
| 667      | .     | 150 | TYR  | CD1  | 133.490    | 0.20        | 3         |
| 668      | .     | 150 | TYR  | CD2  | 133.490    | 0.20        | 3         |
| 669      | .     | 150 | TYR  | CE1  | 118.256    | 0.20        | 3         |
| 670      | .     | 150 | TYR  | CE2  | 118.256    | 0.20        | 3         |
| 671      | .     | 150 | TYR  | N    | 120.403    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 672      | .     | 151 | ARG  | H    | 7.938      | 0.02        | 1         |
| 673      | .     | 151 | ARG  | HA   | 3.923      | 0.02        | 1         |
| 674      | .     | 151 | ARG  | HB2  | 2.075      | 0.02        | 2         |
| 675      | .     | 151 | ARG  | HB3  | 1.947      | 0.02        | 2         |
| 676      | .     | 151 | ARG  | HG2  | 2.020      | 0.02        | 2         |
| 677      | .     | 151 | ARG  | HG3  | 1.743      | 0.02        | 2         |
| 678      | .     | 151 | ARG  | HD2  | 3.276      | 0.02        | 2         |
| 679      | .     | 151 | ARG  | HD3  | 3.368      | 0.02        | 2         |
| 680      | .     | 151 | ARG  | CA   | 59.927     | 0.20        | 1         |
| 681      | .     | 151 | ARG  | CB   | 29.978     | 0.20        | 1         |
| 682      | .     | 151 | ARG  | CG   | 28.328     | 0.20        | 1         |
| 683      | .     | 151 | ARG  | CD   | 43.382     | 0.20        | 1         |
| 684      | .     | 151 | ARG  | N    | 117.923    | 0.20        | 1         |
| 685      | .     | 152 | GLU  | H    | 8.045      | 0.02        | 1         |
| 686      | .     | 152 | GLU  | HA   | 4.064      | 0.02        | 1         |
| 687      | .     | 152 | GLU  | HB2  | 1.884      | 0.02        | 2         |
| 688      | .     | 152 | GLU  | HB3  | 1.899      | 0.02        | 2         |
| 689      | .     | 152 | GLU  | HG2  | 2.199      | 0.02        | 2         |
| 690      | .     | 152 | GLU  | HG3  | 2.419      | 0.02        | 2         |
| 691      | .     | 152 | GLU  | CA   | 58.098     | 0.20        | 1         |
| 692      | .     | 152 | GLU  | CB   | 29.979     | 0.20        | 1         |
| 693      | .     | 152 | GLU  | CG   | 36.545     | 0.20        | 1         |
| 694      | .     | 152 | GLU  | N    | 116.389    | 0.20        | 1         |
| 695      | .     | 153 | ASN  | H    | 7.539      | 0.02        | 1         |
| 696      | .     | 153 | ASN  | HA   | 4.371      | 0.02        | 1         |
| 697      | .     | 153 | ASN  | HB2  | 2.157      | 0.02        | 2         |
| 698      | .     | 153 | ASN  | HB3  | 2.157      | 0.02        | 2         |
| 699      | .     | 153 | ASN  | HD21 | 6.793      | 0.02        | 2         |
| 700      | .     | 153 | ASN  | HD22 | 6.537      | 0.02        | 2         |
| 701      | .     | 153 | ASN  | CA   | 54.896     | 0.20        | 1         |
| 702      | .     | 153 | ASN  | CB   | 41.206     | 0.20        | 1         |
| 703      | .     | 153 | ASN  | N    | 114.747    | 0.20        | 1         |
| 704      | .     | 153 | ASN  | ND2  | 117.123    | 0.20        | 1         |
| 705      | .     | 154 | MET  | H    | 8.021      | 0.02        | 1         |
| 706      | .     | 154 | MET  | HA   | 3.432      | 0.02        | 1         |
| 707      | .     | 154 | MET  | HB2  | 1.318      | 0.02        | 2         |
| 708      | .     | 154 | MET  | HB3  | 1.665      | 0.02        | 2         |
| 709      | .     | 154 | MET  | HG2  | 2.536      | 0.02        | 2         |
| 710      | .     | 154 | MET  | HG3  | 2.144      | 0.02        | 2         |
| 711      | .     | 154 | MET  | HE   | 2.006      | 0.02        | 1         |
| 712      | .     | 154 | MET  | HE   | 2.006      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 713      | .     | 154 | MET  | HE   | 2.006      | 0.02        | 1         |
| 714      | .     | 154 | MET  | CA   | 59.245     | 0.20        | 1         |
| 715      | .     | 154 | MET  | CB   | 30.366     | 0.20        | 1         |
| 716      | .     | 154 | MET  | CG   | 30.604     | 0.20        | 1         |
| 717      | .     | 154 | MET  | CE   | 17.697     | 0.20        | 1         |
| 718      | .     | 154 | MET  | N    | 119.156    | 0.20        | 1         |
| 719      | .     | 155 | HIS  | H    | 7.972      | 0.02        | 1         |
| 720      | .     | 155 | HIS  | HA   | 4.197      | 0.02        | 1         |
| 721      | .     | 155 | HIS  | HB2  | 3.247      | 0.02        | 2         |
| 722      | .     | 155 | HIS  | HB3  | 2.967      | 0.02        | 2         |
| 723      | .     | 155 | HIS  | HD2  | 7.386      | 0.02        | 1         |
| 724      | .     | 155 | HIS  | CA   | 57.795     | 0.20        | 1         |
| 725      | .     | 155 | HIS  | CB   | 29.025     | 0.20        | 1         |
| 726      | .     | 155 | HIS  | CD2  | 120.157    | 0.20        | 1         |
| 727      | .     | 155 | HIS  | N    | 115.717    | 0.20        | 1         |
| 728      | .     | 156 | ARG  | H    | 7.494      | 0.02        | 1         |
| 729      | .     | 156 | ARG  | HA   | 4.092      | 0.02        | 1         |
| 730      | .     | 156 | ARG  | HB2  | 1.395      | 0.02        | 2         |
| 731      | .     | 156 | ARG  | HB3  | 2.092      | 0.02        | 2         |
| 732      | .     | 156 | ARG  | HG2  | 1.369      | 0.02        | 2         |
| 733      | .     | 156 | ARG  | HG3  | 0.313      | 0.02        | 2         |
| 734      | .     | 156 | ARG  | HD2  | 3.076      | 0.02        | 2         |
| 735      | .     | 156 | ARG  | HD3  | 3.246      | 0.02        | 2         |
| 736      | .     | 156 | ARG  | CA   | 56.255     | 0.20        | 1         |
| 737      | .     | 156 | ARG  | CB   | 30.668     | 0.20        | 1         |
| 738      | .     | 156 | ARG  | CG   | 27.304     | 0.20        | 1         |
| 739      | .     | 156 | ARG  | CD   | 44.128     | 0.20        | 1         |
| 740      | .     | 156 | ARG  | N    | 118.743    | 0.20        | 1         |
| 741      | .     | 157 | TYR  | H    | 7.417      | 0.02        | 1         |
| 742      | .     | 157 | TYR  | HA   | 5.021      | 0.02        | 1         |
| 743      | .     | 157 | TYR  | HB2  | 3.117      | 0.02        | 2         |
| 744      | .     | 157 | TYR  | HB3  | 3.116      | 0.02        | 2         |
| 745      | .     | 157 | TYR  | HD1  | 6.887      | 0.02        | 3         |
| 746      | .     | 157 | TYR  | HD2  | 6.887      | 0.02        | 3         |
| 747      | .     | 157 | TYR  | HE1  | 6.554      | 0.02        | 3         |
| 748      | .     | 157 | TYR  | HE2  | 6.554      | 0.02        | 3         |
| 749      | .     | 157 | TYR  | CA   | 52.636     | 0.20        | 1         |
| 750      | .     | 157 | TYR  | CB   | 35.138     | 0.20        | 1         |
| 751      | .     | 157 | TYR  | CD1  | 131.268    | 0.20        | 3         |
| 752      | .     | 157 | TYR  | CD2  | 131.272    | 0.20        | 3         |
| 753      | .     | 157 | TYR  | CE1  | 117.029    | 0.20        | 3         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 754      | .     | 157 | TYR  | CE2  | 117.029    | 0.20        | 3         |
| 755      | .     | 157 | TYR  | N    | 121.155    | 0.20        | 1         |
| 756      | .     | 158 | PRO  | HA   | 4.488      | 0.02        | 1         |
| 757      | .     | 158 | PRO  | HB2  | 1.720      | 0.02        | 2         |
| 758      | .     | 158 | PRO  | HB3  | 2.069      | 0.02        | 2         |
| 759      | .     | 158 | PRO  | HG2  | 1.604      | 0.02        | 2         |
| 760      | .     | 158 | PRO  | HG3  | 1.197      | 0.02        | 2         |
| 761      | .     | 158 | PRO  | HD2  | 3.179      | 0.02        | 2         |
| 762      | .     | 158 | PRO  | HD3  | 3.153      | 0.02        | 2         |
| 763      | .     | 158 | PRO  | CA   | 63.628     | 0.20        | 1         |
| 764      | .     | 158 | PRO  | CB   | 32.549     | 0.20        | 1         |
| 765      | .     | 158 | PRO  | CG   | 27.461     | 0.20        | 1         |
| 766      | .     | 158 | PRO  | CD   | 49.883     | 0.20        | 1         |
| 767      | .     | 159 | ASN  | H    | 8.470      | 0.02        | 1         |
| 768      | .     | 159 | ASN  | HA   | 4.718      | 0.02        | 1         |
| 769      | .     | 159 | ASN  | HB2  | 2.405      | 0.02        | 2         |
| 770      | .     | 159 | ASN  | HB3  | 2.405      | 0.02        | 2         |
| 771      | .     | 159 | ASN  | HD21 | 6.749      | 0.02        | 2         |
| 772      | .     | 159 | ASN  | HD22 | 7.445      | 0.02        | 2         |
| 773      | .     | 159 | ASN  | CA   | 51.862     | 0.20        | 1         |
| 774      | .     | 159 | ASN  | CB   | 38.212     | 0.20        | 1         |
| 775      | .     | 159 | ASN  | N    | 115.787    | 0.20        | 1         |
| 776      | .     | 159 | ASN  | ND2  | 109.022    | 0.20        | 1         |
| 777      | .     | 160 | GLN  | H    | 7.200      | 0.02        | 1         |
| 778      | .     | 160 | GLN  | HA   | 4.531      | 0.02        | 1         |
| 779      | .     | 160 | GLN  | HB2  | 1.694      | 0.02        | 2         |
| 780      | .     | 160 | GLN  | HB3  | 1.979      | 0.02        | 2         |
| 781      | .     | 160 | GLN  | HG2  | 2.034      | 0.02        | 2         |
| 782      | .     | 160 | GLN  | HG3  | 2.150      | 0.02        | 2         |
| 783      | .     | 160 | GLN  | HE21 | 7.906      | 0.02        | 2         |
| 784      | .     | 160 | GLN  | HE22 | 6.936      | 0.02        | 2         |
| 785      | .     | 160 | GLN  | CA   | 54.311     | 0.20        | 1         |
| 786      | .     | 160 | GLN  | CB   | 33.891     | 0.20        | 1         |
| 787      | .     | 160 | GLN  | CG   | 34.260     | 0.20        | 1         |
| 788      | .     | 160 | GLN  | N    | 113.794    | 0.20        | 1         |
| 789      | .     | 160 | GLN  | NE2  | 112.558    | 0.20        | 1         |
| 790      | .     | 161 | VAL  | H    | 8.455      | 0.02        | 1         |
| 791      | .     | 161 | VAL  | HA   | 4.887      | 0.02        | 1         |
| 792      | .     | 161 | VAL  | HB   | 2.608      | 0.02        | 1         |
| 793      | .     | 161 | VAL  | HG1  | 0.953      | 0.02        | 2         |
| 794      | .     | 161 | VAL  | HG1  | 0.953      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 795      | .     | 161 | VAL  | HG1  | 0.953      | 0.02        | 2         |
| 796      | .     | 161 | VAL  | HG2  | 0.746      | 0.02        | 2         |
| 797      | .     | 161 | VAL  | HG2  | 0.746      | 0.02        | 2         |
| 798      | .     | 161 | VAL  | HG2  | 0.746      | 0.02        | 2         |
| 799      | .     | 161 | VAL  | CA   | 58.796     | 0.20        | 1         |
| 800      | .     | 161 | VAL  | CB   | 34.042     | 0.20        | 1         |
| 801      | .     | 161 | VAL  | CG1  | 23.770     | 0.20        | 2         |
| 802      | .     | 161 | VAL  | CG2  | 18.428     | 0.20        | 2         |
| 803      | .     | 161 | VAL  | N    | 112.453    | 0.20        | 1         |
| 804      | .     | 162 | TYR  | H    | 8.478      | 0.02        | 1         |
| 805      | .     | 162 | TYR  | HA   | 5.537      | 0.02        | 1         |
| 806      | .     | 162 | TYR  | HB2  | 2.497      | 0.02        | 2         |
| 807      | .     | 162 | TYR  | HB3  | 2.642      | 0.02        | 2         |
| 808      | .     | 162 | TYR  | HD1  | 6.925      | 0.02        | 3         |
| 809      | .     | 162 | TYR  | HD2  | 6.926      | 0.02        | 3         |
| 810      | .     | 162 | TYR  | HE1  | 6.757      | 0.02        | 3         |
| 811      | .     | 162 | TYR  | HE2  | 6.757      | 0.02        | 3         |
| 812      | .     | 162 | TYR  | CA   | 57.056     | 0.20        | 1         |
| 813      | .     | 162 | TYR  | CB   | 41.984     | 0.20        | 1         |
| 814      | .     | 162 | TYR  | CD1  | 133.376    | 0.20        | 3         |
| 815      | .     | 162 | TYR  | CD2  | 133.383    | 0.20        | 3         |
| 816      | .     | 162 | TYR  | CE1  | 117.963    | 0.20        | 3         |
| 817      | .     | 162 | TYR  | CE2  | 117.963    | 0.20        | 3         |
| 818      | .     | 162 | TYR  | N    | 121.224    | 0.20        | 1         |
| 819      | .     | 163 | TYR  | H    | 8.557      | 0.02        | 1         |
| 820      | .     | 163 | TYR  | HA   | 4.738      | 0.02        | 1         |
| 821      | .     | 163 | TYR  | HB2  | 2.882      | 0.02        | 2         |
| 822      | .     | 163 | TYR  | HB3  | 2.840      | 0.02        | 2         |
| 823      | .     | 163 | TYR  | HD1  | 6.949      | 0.02        | 3         |
| 824      | .     | 163 | TYR  | HD2  | 6.950      | 0.02        | 3         |
| 825      | .     | 163 | TYR  | HE1  | 6.460      | 0.02        | 3         |
| 826      | .     | 163 | TYR  | HE2  | 6.460      | 0.02        | 3         |
| 827      | .     | 163 | TYR  | CA   | 55.915     | 0.20        | 1         |
| 828      | .     | 163 | TYR  | CB   | 40.324     | 0.20        | 1         |
| 829      | .     | 163 | TYR  | CD1  | 133.587    | 0.20        | 3         |
| 830      | .     | 163 | TYR  | CD2  | 133.593    | 0.20        | 3         |
| 831      | .     | 163 | TYR  | CE1  | 117.788    | 0.20        | 3         |
| 832      | .     | 163 | TYR  | CE2  | 117.788    | 0.20        | 3         |
| 833      | .     | 163 | TYR  | N    | 110.937    | 0.20        | 1         |
| 834      | .     | 166 | MET  | H    | 8.973      | 0.02        | 1         |
| 835      | .     | 166 | MET  | HA   | 4.445      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 836      | .     | 166 | MET  | HB2  | 2.287      | 0.02        | 2         |
| 837      | .     | 166 | MET  | HB3  | 2.211      | 0.02        | 2         |
| 838      | .     | 166 | MET  | HG2  | 1.817      | 0.02        | 2         |
| 839      | .     | 166 | MET  | HG3  | 1.740      | 0.02        | 2         |
| 840      | .     | 166 | MET  | HE   | 1.594      | 0.02        | 1         |
| 841      | .     | 166 | MET  | HE   | 1.594      | 0.02        | 1         |
| 842      | .     | 166 | MET  | HE   | 1.594      | 0.02        | 1         |
| 843      | .     | 166 | MET  | CA   | 57.496     | 0.20        | 1         |
| 844      | .     | 166 | MET  | CB   | 32.380     | 0.20        | 1         |
| 845      | .     | 166 | MET  | CG   | 32.770     | 0.20        | 1         |
| 846      | .     | 166 | MET  | CE   | 17.225     | 0.20        | 1         |
| 847      | .     | 166 | MET  | N    | 120.974    | 0.20        | 1         |
| 848      | .     | 168 | GLU  | H    | 8.422      | 0.02        | 1         |
| 849      | .     | 168 | GLU  | HA   | 4.336      | 0.02        | 1         |
| 850      | .     | 168 | GLU  | HB2  | 2.004      | 0.02        | 2         |
| 851      | .     | 168 | GLU  | HB3  | 1.956      | 0.02        | 2         |
| 852      | .     | 168 | GLU  | HG2  | 2.564      | 0.02        | 2         |
| 853      | .     | 168 | GLU  | HG3  | 2.564      | 0.02        | 2         |
| 854      | .     | 168 | GLU  | CA   | 56.085     | 0.20        | 1         |
| 855      | .     | 168 | GLU  | CB   | 32.928     | 0.20        | 1         |
| 856      | .     | 168 | GLU  | CG   | 32.121     | 0.20        | 1         |
| 857      | .     | 168 | GLU  | N    | 126.021    | 0.20        | 1         |
| 858      | .     | 169 | TYR  | H    | 8.382      | 0.02        | 1         |
| 859      | .     | 169 | TYR  | HA   | 4.254      | 0.02        | 1         |
| 860      | .     | 169 | TYR  | CA   | 56.839     | 0.20        | 1         |
| 861      | .     | 169 | TYR  | N    | 121.023    | 0.20        | 1         |
| 862      | .     | 170 | SER  | H    | 8.174      | 0.02        | 1         |
| 863      | .     | 170 | SER  | HA   | 4.360      | 0.02        | 1         |
| 864      | .     | 170 | SER  | HB2  | 4.770      | 0.02        | 2         |
| 865      | .     | 170 | SER  | HB3  | 4.720      | 0.02        | 2         |
| 866      | .     | 170 | SER  | CA   | 58.400     | 0.20        | 1         |
| 867      | .     | 170 | SER  | CB   | 63.900     | 0.20        | 1         |
| 868      | .     | 170 | SER  | N    | 115.552    | 0.20        | 1         |
| 869      | .     | 172 | GLN  | H    | 8.654      | 0.02        | 1         |
| 870      | .     | 172 | GLN  | HB2  | 1.609      | 0.02        | 2         |
| 871      | .     | 172 | GLN  | HB3  | 1.609      | 0.02        | 2         |
| 872      | .     | 172 | GLN  | HG2  | 1.830      | 0.02        | 2         |
| 873      | .     | 172 | GLN  | HG3  | 1.762      | 0.02        | 2         |
| 874      | .     | 172 | GLN  | HE21 | 7.215      | 0.02        | 2         |
| 875      | .     | 172 | GLN  | HE22 | 7.099      | 0.02        | 2         |
| 876      | .     | 172 | GLN  | CB   | 29.100     | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 877      | .     | 172 | GLN  | CG   | 32.382     | 0.20        | 1         |
| 878      | .     | 172 | GLN  | N    | 120.356    | 0.20        | 1         |
| 879      | .     | 172 | GLN  | NE2  | 111.787    | 0.20        | 1         |
| 880      | .     | 173 | ASN  | H    | 8.340      | 0.02        | 1         |
| 881      | .     | 173 | ASN  | HA   | 4.234      | 0.02        | 1         |
| 882      | .     | 173 | ASN  | HB2  | 2.742      | 0.02        | 2         |
| 883      | .     | 173 | ASN  | HB3  | 2.670      | 0.02        | 2         |
| 884      | .     | 173 | ASN  | HD21 | 7.571      | 0.02        | 2         |
| 885      | .     | 173 | ASN  | HD22 | 6.932      | 0.02        | 2         |
| 886      | .     | 173 | ASN  | CA   | 56.513     | 0.20        | 1         |
| 887      | .     | 173 | ASN  | CB   | 38.036     | 0.20        | 1         |
| 888      | .     | 173 | ASN  | N    | 116.773    | 0.20        | 1         |
| 889      | .     | 173 | ASN  | ND2  | 112.743    | 0.20        | 1         |
| 890      | .     | 174 | ASN  | H    | 8.610      | 0.02        | 1         |
| 891      | .     | 174 | ASN  | HA   | 4.549      | 0.02        | 1         |
| 892      | .     | 174 | ASN  | HB2  | 3.039      | 0.02        | 2         |
| 893      | .     | 174 | ASN  | HB3  | 2.932      | 0.02        | 2         |
| 894      | .     | 174 | ASN  | HD21 | 7.093      | 0.02        | 2         |
| 895      | .     | 174 | ASN  | HD22 | 7.674      | 0.02        | 2         |
| 896      | .     | 174 | ASN  | CA   | 55.945     | 0.20        | 1         |
| 897      | .     | 174 | ASN  | CB   | 37.972     | 0.20        | 1         |
| 898      | .     | 174 | ASN  | N    | 118.447    | 0.20        | 1         |
| 899      | .     | 174 | ASN  | ND2  | 112.231    | 0.20        | 1         |
| 900      | .     | 175 | PHE  | HD1  | 7.670      | 0.02        | 3         |
| 901      | .     | 175 | PHE  | HD2  | 7.670      | 0.02        | 3         |
| 902      | .     | 175 | PHE  | HE1  | 6.727      | 0.02        | 3         |
| 903      | .     | 175 | PHE  | HE2  | 6.727      | 0.02        | 3         |
| 904      | .     | 175 | PHE  | HZ   | 7.298      | 0.02        | 1         |
| 905      | .     | 175 | PHE  | CD1  | 131.715    | 0.20        | 3         |
| 906      | .     | 175 | PHE  | CD2  | 131.713    | 0.20        | 3         |
| 907      | .     | 175 | PHE  | CE1  | 129.085    | 0.20        | 3         |
| 908      | .     | 175 | PHE  | CE2  | 129.076    | 0.20        | 3         |
| 909      | .     | 175 | PHE  | CZ   | 133.149    | 0.20        | 1         |
| 910      | .     | 176 | VAL  | H    | 8.924      | 0.02        | 1         |
| 911      | .     | 176 | VAL  | HA   | 3.529      | 0.02        | 1         |
| 912      | .     | 176 | VAL  | HB   | 2.212      | 0.02        | 1         |
| 913      | .     | 176 | VAL  | HG1  | 1.077      | 0.02        | 2         |
| 914      | .     | 176 | VAL  | HG1  | 1.077      | 0.02        | 2         |
| 915      | .     | 176 | VAL  | HG1  | 1.077      | 0.02        | 2         |
| 916      | .     | 176 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 917      | .     | 176 | VAL  | HG2  | 0.957      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 918      | .     | 176 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 919      | .     | 176 | VAL  | CA   | 67.799     | 0.20        | 1         |
| 920      | .     | 176 | VAL  | CB   | 32.184     | 0.20        | 1         |
| 921      | .     | 176 | VAL  | CG1  | 24.751     | 0.20        | 2         |
| 922      | .     | 176 | VAL  | CG2  | 21.722     | 0.20        | 2         |
| 923      | .     | 176 | VAL  | N    | 120.257    | 0.20        | 1         |
| 924      | .     | 177 | HIS  | H    | 8.309      | 0.02        | 1         |
| 925      | .     | 177 | HIS  | HA   | 4.317      | 0.02        | 1         |
| 926      | .     | 177 | HIS  | HB2  | 3.381      | 0.02        | 2         |
| 927      | .     | 177 | HIS  | HB3  | 3.332      | 0.02        | 2         |
| 928      | .     | 177 | HIS  | HD2  | 7.309      | 0.02        | 1         |
| 929      | .     | 177 | HIS  | HE1  | 8.612      | 0.02        | 1         |
| 930      | .     | 177 | HIS  | CA   | 59.531     | 0.20        | 1         |
| 931      | .     | 177 | HIS  | CB   | 28.349     | 0.20        | 1         |
| 932      | .     | 177 | HIS  | CD2  | 119.973    | 0.20        | 1         |
| 933      | .     | 177 | HIS  | CE1  | 136.305    | 0.20        | 1         |
| 934      | .     | 177 | HIS  | N    | 116.859    | 0.20        | 1         |
| 935      | .     | 178 | ASP  | H    | 7.769      | 0.02        | 1         |
| 936      | .     | 178 | ASP  | HA   | 4.523      | 0.02        | 1         |
| 937      | .     | 178 | ASP  | HB2  | 2.960      | 0.02        | 2         |
| 938      | .     | 178 | ASP  | HB3  | 2.821      | 0.02        | 2         |
| 939      | .     | 178 | ASP  | CA   | 57.670     | 0.20        | 1         |
| 940      | .     | 178 | ASP  | CB   | 41.373     | 0.20        | 1         |
| 941      | .     | 178 | ASP  | N    | 118.696    | 0.20        | 1         |
| 942      | .     | 179 | CYS  | H    | 8.064      | 0.02        | 1         |
| 943      | .     | 179 | CYS  | HA   | 4.661      | 0.02        | 1         |
| 944      | .     | 179 | CYS  | HB2  | 3.000      | 0.02        | 2         |
| 945      | .     | 179 | CYS  | HB3  | 3.371      | 0.02        | 2         |
| 946      | .     | 179 | CYS  | CA   | 58.579     | 0.20        | 1         |
| 947      | .     | 179 | CYS  | CB   | 40.663     | 0.20        | 1         |
| 948      | .     | 179 | CYS  | N    | 119.374    | 0.20        | 1         |
| 949      | .     | 180 | VAL  | H    | 9.108      | 0.02        | 1         |
| 950      | .     | 180 | VAL  | HA   | 3.676      | 0.02        | 1         |
| 951      | .     | 180 | VAL  | HB   | 2.211      | 0.02        | 1         |
| 952      | .     | 180 | VAL  | HG1  | 0.883      | 0.02        | 2         |
| 953      | .     | 180 | VAL  | HG1  | 0.883      | 0.02        | 2         |
| 954      | .     | 180 | VAL  | HG1  | 0.883      | 0.02        | 2         |
| 955      | .     | 180 | VAL  | HG2  | 1.085      | 0.02        | 2         |
| 956      | .     | 180 | VAL  | HG2  | 1.085      | 0.02        | 2         |
| 957      | .     | 180 | VAL  | HG2  | 1.085      | 0.02        | 2         |
| 958      | .     | 180 | VAL  | CA   | 66.375     | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 959      | .     | 180 | VAL  | CB   | 32.137     | 0.20        | 1         |
| 960      | .     | 180 | VAL  | CG1  | 21.224     | 0.20        | 2         |
| 961      | .     | 180 | VAL  | CG2  | 23.408     | 0.20        | 2         |
| 962      | .     | 180 | VAL  | N    | 124.885    | 0.20        | 1         |
| 963      | .     | 181 | ASN  | H    | 7.653      | 0.02        | 1         |
| 964      | .     | 181 | ASN  | HA   | 4.313      | 0.02        | 1         |
| 965      | .     | 181 | ASN  | HB2  | 2.760      | 0.02        | 2         |
| 966      | .     | 181 | ASN  | HB3  | 2.835      | 0.02        | 2         |
| 967      | .     | 181 | ASN  | HD21 | 6.744      | 0.02        | 2         |
| 968      | .     | 181 | ASN  | HD22 | 7.608      | 0.02        | 2         |
| 969      | .     | 181 | ASN  | CA   | 56.517     | 0.20        | 1         |
| 970      | .     | 181 | ASN  | CB   | 38.805     | 0.20        | 1         |
| 971      | .     | 181 | ASN  | N    | 116.341    | 0.20        | 1         |
| 972      | .     | 181 | ASN  | ND2  | 112.006    | 0.20        | 1         |
| 973      | .     | 182 | ILE  | H    | 8.725      | 0.02        | 1         |
| 974      | .     | 182 | ILE  | HA   | 3.770      | 0.02        | 1         |
| 975      | .     | 182 | ILE  | HB   | 1.547      | 0.02        | 1         |
| 976      | .     | 182 | ILE  | HG12 | 0.764      | 0.02        | 2         |
| 977      | .     | 182 | ILE  | HG13 | 0.883      | 0.02        | 2         |
| 978      | .     | 182 | ILE  | HG2  | 0.298      | 0.02        | 1         |
| 979      | .     | 182 | ILE  | HG2  | 0.298      | 0.02        | 1         |
| 980      | .     | 182 | ILE  | HG2  | 0.298      | 0.02        | 1         |
| 981      | .     | 182 | ILE  | HD1  | 0.408      | 0.02        | 1         |
| 982      | .     | 182 | ILE  | HD1  | 0.408      | 0.02        | 1         |
| 983      | .     | 182 | ILE  | HD1  | 0.408      | 0.02        | 1         |
| 984      | .     | 182 | ILE  | CA   | 62.294     | 0.20        | 1         |
| 985      | .     | 182 | ILE  | CB   | 36.868     | 0.20        | 1         |
| 986      | .     | 182 | ILE  | CG1  | 27.801     | 0.20        | 1         |
| 987      | .     | 182 | ILE  | CG2  | 18.699     | 0.20        | 1         |
| 988      | .     | 182 | ILE  | CD1  | 11.930     | 0.20        | 1         |
| 989      | .     | 182 | ILE  | N    | 118.794    | 0.20        | 1         |
| 990      | .     | 183 | THR  | H    | 8.136      | 0.02        | 1         |
| 991      | .     | 183 | THR  | HA   | 4.060      | 0.02        | 1         |
| 992      | .     | 183 | THR  | HB   | 4.495      | 0.02        | 1         |
| 993      | .     | 183 | THR  | HG2  | 1.516      | 0.02        | 1         |
| 994      | .     | 183 | THR  | HG2  | 1.516      | 0.02        | 1         |
| 995      | .     | 183 | THR  | HG2  | 1.516      | 0.02        | 1         |
| 996      | .     | 183 | THR  | CA   | 68.958     | 0.20        | 1         |
| 997      | .     | 183 | THR  | CB   | 68.113     | 0.20        | 1         |
| 998      | .     | 183 | THR  | CG2  | 22.238     | 0.20        | 1         |
| 999      | .     | 183 | THR  | N    | 118.418    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1000     | .     | 184 | ILE  | H    | 8.648      | 0.02        | 1         |
| 1001     | .     | 184 | ILE  | HA   | 3.675      | 0.02        | 1         |
| 1002     | .     | 184 | ILE  | HB   | 1.942      | 0.02        | 1         |
| 1003     | .     | 184 | ILE  | HG12 | 1.528      | 0.02        | 2         |
| 1004     | .     | 184 | ILE  | HG13 | 1.820      | 0.02        | 2         |
| 1005     | .     | 184 | ILE  | HG2  | 0.921      | 0.02        | 1         |
| 1006     | .     | 184 | ILE  | HG2  | 0.921      | 0.02        | 1         |
| 1007     | .     | 184 | ILE  | HG2  | 0.921      | 0.02        | 1         |
| 1008     | .     | 184 | ILE  | HD1  | 0.802      | 0.02        | 1         |
| 1009     | .     | 184 | ILE  | HD1  | 0.802      | 0.02        | 1         |
| 1010     | .     | 184 | ILE  | HD1  | 0.802      | 0.02        | 1         |
| 1011     | .     | 184 | ILE  | CA   | 66.416     | 0.20        | 1         |
| 1012     | .     | 184 | ILE  | CB   | 37.714     | 0.20        | 1         |
| 1013     | .     | 184 | ILE  | CG1  | 30.753     | 0.20        | 1         |
| 1014     | .     | 184 | ILE  | CG2  | 16.972     | 0.20        | 1         |
| 1015     | .     | 184 | ILE  | CD1  | 14.236     | 0.20        | 1         |
| 1016     | .     | 184 | ILE  | N    | 121.653    | 0.20        | 1         |
| 1017     | .     | 185 | LYS  | H    | 7.844      | 0.02        | 1         |
| 1018     | .     | 185 | LYS  | HA   | 4.038      | 0.02        | 1         |
| 1019     | .     | 185 | LYS  | HB2  | 1.895      | 0.02        | 2         |
| 1020     | .     | 185 | LYS  | HB3  | 1.895      | 0.02        | 2         |
| 1021     | .     | 185 | LYS  | HG2  | 1.450      | 0.02        | 2         |
| 1022     | .     | 185 | LYS  | HG3  | 1.357      | 0.02        | 2         |
| 1023     | .     | 185 | LYS  | HD2  | 1.603      | 0.02        | 2         |
| 1024     | .     | 185 | LYS  | HD3  | 1.657      | 0.02        | 2         |
| 1025     | .     | 185 | LYS  | HE2  | 2.967      | 0.02        | 2         |
| 1026     | .     | 185 | LYS  | HE3  | 2.905      | 0.02        | 2         |
| 1027     | .     | 185 | LYS  | CA   | 59.940     | 0.20        | 1         |
| 1028     | .     | 185 | LYS  | CB   | 32.239     | 0.20        | 1         |
| 1029     | .     | 185 | LYS  | CG   | 24.723     | 0.20        | 1         |
| 1030     | .     | 185 | LYS  | CD   | 29.020     | 0.20        | 1         |
| 1031     | .     | 185 | LYS  | CE   | 41.900     | 0.20        | 1         |
| 1032     | .     | 185 | LYS  | N    | 122.998    | 0.20        | 1         |
| 1033     | .     | 187 | HIS  | H    | 8.291      | 0.02        | 1         |
| 1034     | .     | 187 | HIS  | HA   | 4.606      | 0.02        | 1         |
| 1035     | .     | 187 | HIS  | HB2  | 3.269      | 0.02        | 2         |
| 1036     | .     | 187 | HIS  | HB3  | 3.227      | 0.02        | 2         |
| 1037     | .     | 187 | HIS  | HD2  | 7.219      | 0.02        | 1         |
| 1038     | .     | 187 | HIS  | CA   | 58.999     | 0.20        | 1         |
| 1039     | .     | 187 | HIS  | CB   | 30.941     | 0.20        | 1         |
| 1040     | .     | 187 | HIS  | CD2  | 120.058    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1041     | .     | 187 | HIS  | N    | 118.510    | 0.20        | 1         |
| 1042     | .     | 188 | THR  | H    | 8.216      | 0.02        | 1         |
| 1043     | .     | 188 | THR  | HA   | 3.991      | 0.02        | 1         |
| 1044     | .     | 188 | THR  | HB   | 4.159      | 0.02        | 1         |
| 1045     | .     | 188 | THR  | HG2  | 1.253      | 0.02        | 1         |
| 1046     | .     | 188 | THR  | HG2  | 1.253      | 0.02        | 1         |
| 1047     | .     | 188 | THR  | HG2  | 1.253      | 0.02        | 1         |
| 1048     | .     | 188 | THR  | CA   | 65.422     | 0.20        | 1         |
| 1049     | .     | 188 | THR  | CB   | 69.112     | 0.20        | 1         |
| 1050     | .     | 188 | THR  | CG2  | 21.135     | 0.20        | 1         |
| 1051     | .     | 188 | THR  | N    | 113.634    | 0.20        | 1         |
| 1052     | .     | 189 | VAL  | H    | 7.994      | 0.02        | 1         |
| 1053     | .     | 189 | VAL  | HA   | 3.993      | 0.02        | 1         |
| 1054     | .     | 189 | VAL  | HB   | 2.212      | 0.02        | 1         |
| 1055     | .     | 189 | VAL  | HG1  | 1.029      | 0.02        | 2         |
| 1056     | .     | 189 | VAL  | HG1  | 1.029      | 0.02        | 2         |
| 1057     | .     | 189 | VAL  | HG1  | 1.029      | 0.02        | 2         |
| 1058     | .     | 189 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 1059     | .     | 189 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 1060     | .     | 189 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 1061     | .     | 189 | VAL  | CA   | 65.187     | 0.20        | 1         |
| 1062     | .     | 189 | VAL  | CB   | 32.220     | 0.20        | 1         |
| 1063     | .     | 189 | VAL  | CG1  | 21.688     | 0.20        | 2         |
| 1064     | .     | 189 | VAL  | CG2  | 21.038     | 0.20        | 2         |
| 1065     | .     | 189 | VAL  | N    | 122.245    | 0.20        | 1         |
| 1066     | .     | 190 | THR  | H    | 8.094      | 0.02        | 1         |
| 1067     | .     | 190 | THR  | HA   | 4.213      | 0.02        | 1         |
| 1068     | .     | 190 | THR  | HB   | 4.269      | 0.02        | 1         |
| 1069     | .     | 190 | THR  | HG2  | 1.276      | 0.02        | 1         |
| 1070     | .     | 190 | THR  | HG2  | 1.276      | 0.02        | 1         |
| 1071     | .     | 190 | THR  | HG2  | 1.276      | 0.02        | 1         |
| 1072     | .     | 190 | THR  | CA   | 64.338     | 0.20        | 1         |
| 1073     | .     | 190 | THR  | CB   | 69.331     | 0.20        | 1         |
| 1074     | .     | 190 | THR  | CG2  | 21.727     | 0.20        | 1         |
| 1075     | .     | 190 | THR  | N    | 115.242    | 0.20        | 1         |
| 1076     | .     | 191 | THR  | H    | 7.998      | 0.02        | 1         |
| 1077     | .     | 191 | THR  | HA   | 4.189      | 0.02        | 1         |
| 1078     | .     | 191 | THR  | HB   | 4.267      | 0.02        | 1         |
| 1079     | .     | 191 | THR  | HG2  | 0.925      | 0.02        | 1         |
| 1080     | .     | 191 | THR  | HG2  | 0.925      | 0.02        | 1         |
| 1081     | .     | 191 | THR  | HG2  | 0.925      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1082     | .     | 191 | THR  | CA   | 64.196     | 0.20        | 1         |
| 1083     | .     | 191 | THR  | CB   | 69.248     | 0.20        | 1         |
| 1084     | .     | 191 | THR  | CG2  | 19.283     | 0.20        | 1         |
| 1085     | .     | 191 | THR  | N    | 114.733    | 0.20        | 1         |
| 1086     | .     | 192 | THR  | H    | 8.166      | 0.02        | 1         |
| 1087     | .     | 192 | THR  | HA   | 4.381      | 0.02        | 1         |
| 1088     | .     | 192 | THR  | HB   | 4.356      | 0.02        | 1         |
| 1089     | .     | 192 | THR  | HG2  | 1.294      | 0.02        | 1         |
| 1090     | .     | 192 | THR  | HG2  | 1.294      | 0.02        | 1         |
| 1091     | .     | 192 | THR  | HG2  | 1.294      | 0.02        | 1         |
| 1092     | .     | 192 | THR  | CA   | 64.356     | 0.20        | 1         |
| 1093     | .     | 192 | THR  | CB   | 69.230     | 0.20        | 1         |
| 1094     | .     | 192 | THR  | CG2  | 21.602     | 0.20        | 1         |
| 1095     | .     | 192 | THR  | N    | 117.067    | 0.20        | 1         |
| 1096     | .     | 193 | THR  | H    | 7.882      | 0.02        | 1         |
| 1097     | .     | 193 | THR  | HA   | 4.229      | 0.02        | 1         |
| 1098     | .     | 193 | THR  | HB   | 4.295      | 0.02        | 1         |
| 1099     | .     | 193 | THR  | HG2  | 1.231      | 0.02        | 1         |
| 1100     | .     | 193 | THR  | HG2  | 1.231      | 0.02        | 1         |
| 1101     | .     | 193 | THR  | HG2  | 1.231      | 0.02        | 1         |
| 1102     | .     | 193 | THR  | CA   | 63.993     | 0.20        | 1         |
| 1103     | .     | 193 | THR  | CB   | 69.233     | 0.20        | 1         |
| 1104     | .     | 193 | THR  | CG2  | 22.102     | 0.20        | 1         |
| 1105     | .     | 193 | THR  | N    | 116.098    | 0.20        | 1         |
| 1106     | .     | 194 | LYS  | H    | 7.708      | 0.02        | 1         |
| 1107     | .     | 194 | LYS  | HA   | 4.341      | 0.02        | 1         |
| 1108     | .     | 194 | LYS  | HB2  | 1.817      | 0.02        | 2         |
| 1109     | .     | 194 | LYS  | HB3  | 1.978      | 0.02        | 2         |
| 1110     | .     | 194 | LYS  | HG2  | 1.454      | 0.02        | 2         |
| 1111     | .     | 194 | LYS  | HG3  | 1.502      | 0.02        | 2         |
| 1112     | .     | 194 | LYS  | HD2  | 1.659      | 0.02        | 2         |
| 1113     | .     | 194 | LYS  | HD3  | 1.659      | 0.02        | 2         |
| 1114     | .     | 194 | LYS  | HE2  | 2.967      | 0.02        | 2         |
| 1115     | .     | 194 | LYS  | HE3  | 2.905      | 0.02        | 2         |
| 1116     | .     | 194 | LYS  | CA   | 56.386     | 0.20        | 1         |
| 1117     | .     | 194 | LYS  | CB   | 32.701     | 0.20        | 1         |
| 1118     | .     | 194 | LYS  | CG   | 25.000     | 0.20        | 1         |
| 1119     | .     | 194 | LYS  | CD   | 29.100     | 0.20        | 1         |
| 1120     | .     | 194 | LYS  | CE   | 41.910     | 0.20        | 1         |
| 1121     | .     | 194 | LYS  | N    | 120.617    | 0.20        | 1         |
| 1122     | .     | 195 | GLY  | H    | 8.026      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1123     | .     | 195 | GLY  | HA2  | 4.074      | 0.02        | 2         |
| 1124     | .     | 195 | GLY  | HA3  | 3.842      | 0.02        | 2         |
| 1125     | .     | 195 | GLY  | CA   | 45.454     | 0.20        | 1         |
| 1126     | .     | 195 | GLY  | N    | 108.539    | 0.20        | 1         |
| 1127     | .     | 196 | GLU  | H    | 7.599      | 0.02        | 1         |
| 1128     | .     | 196 | GLU  | HA   | 4.238      | 0.02        | 1         |
| 1129     | .     | 196 | GLU  | HB2  | 1.607      | 0.02        | 2         |
| 1130     | .     | 196 | GLU  | HB3  | 1.607      | 0.02        | 2         |
| 1131     | .     | 196 | GLU  | HG2  | 2.011      | 0.02        | 2         |
| 1132     | .     | 196 | GLU  | HG3  | 2.087      | 0.02        | 2         |
| 1133     | .     | 196 | GLU  | CA   | 55.820     | 0.20        | 1         |
| 1134     | .     | 196 | GLU  | CB   | 31.008     | 0.20        | 1         |
| 1135     | .     | 196 | GLU  | CG   | 35.919     | 0.20        | 1         |
| 1136     | .     | 196 | GLU  | N    | 120.050    | 0.20        | 1         |
| 1137     | .     | 197 | ASN  | H    | 8.425      | 0.02        | 1         |
| 1138     | .     | 197 | ASN  | HA   | 4.655      | 0.02        | 1         |
| 1139     | .     | 197 | ASN  | HB2  | 2.602      | 0.02        | 2         |
| 1140     | .     | 197 | ASN  | HB3  | 2.668      | 0.02        | 2         |
| 1141     | .     | 197 | ASN  | HD21 | 7.514      | 0.02        | 2         |
| 1142     | .     | 197 | ASN  | HD22 | 6.791      | 0.02        | 2         |
| 1143     | .     | 197 | ASN  | CA   | 52.794     | 0.20        | 1         |
| 1144     | .     | 197 | ASN  | CB   | 40.381     | 0.20        | 1         |
| 1145     | .     | 197 | ASN  | N    | 119.440    | 0.20        | 1         |
| 1146     | .     | 197 | ASN  | ND2  | 113.093    | 0.20        | 1         |
| 1147     | .     | 198 | PHE  | H    | 8.628      | 0.02        | 1         |
| 1148     | .     | 198 | PHE  | HA   | 5.284      | 0.02        | 1         |
| 1149     | .     | 198 | PHE  | HB2  | 2.953      | 0.02        | 2         |
| 1150     | .     | 198 | PHE  | HB3  | 3.158      | 0.02        | 2         |
| 1151     | .     | 198 | PHE  | HD1  | 7.342      | 0.02        | 3         |
| 1152     | .     | 198 | PHE  | HD2  | 7.342      | 0.02        | 3         |
| 1153     | .     | 198 | PHE  | HE1  | 7.459      | 0.02        | 3         |
| 1154     | .     | 198 | PHE  | HE2  | 7.459      | 0.02        | 3         |
| 1155     | .     | 198 | PHE  | HZ   | 7.329      | 0.02        | 1         |
| 1156     | .     | 198 | PHE  | CA   | 56.758     | 0.20        | 1         |
| 1157     | .     | 198 | PHE  | CB   | 40.128     | 0.20        | 1         |
| 1158     | .     | 198 | PHE  | CD1  | 131.514    | 0.20        | 3         |
| 1159     | .     | 198 | PHE  | CD2  | 131.514    | 0.20        | 3         |
| 1160     | .     | 198 | PHE  | CE1  | 130.054    | 0.20        | 3         |
| 1161     | .     | 198 | PHE  | CE2  | 130.054    | 0.20        | 3         |
| 1162     | .     | 198 | PHE  | CZ   | 132.027    | 0.20        | 1         |
| 1163     | .     | 198 | PHE  | N    | 121.719    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1164     | .     | 199 | THR  | H    | 9.520      | 0.02        | 1         |
| 1165     | .     | 199 | THR  | HA   | 4.629      | 0.02        | 1         |
| 1166     | .     | 199 | THR  | HB   | 4.829      | 0.02        | 1         |
| 1167     | .     | 199 | THR  | HG2  | 1.425      | 0.02        | 1         |
| 1168     | .     | 199 | THR  | HG2  | 1.425      | 0.02        | 1         |
| 1169     | .     | 199 | THR  | HG2  | 1.425      | 0.02        | 1         |
| 1170     | .     | 199 | THR  | CA   | 60.470     | 0.20        | 1         |
| 1171     | .     | 199 | THR  | CB   | 72.156     | 0.20        | 1         |
| 1172     | .     | 199 | THR  | CG2  | 21.737     | 0.20        | 1         |
| 1173     | .     | 199 | THR  | N    | 115.920    | 0.20        | 1         |
| 1174     | .     | 200 | GLU  | H    | 9.112      | 0.02        | 1         |
| 1175     | .     | 200 | GLU  | HA   | 4.066      | 0.02        | 1         |
| 1176     | .     | 200 | GLU  | HB2  | 2.136      | 0.02        | 2         |
| 1177     | .     | 200 | GLU  | HB3  | 2.058      | 0.02        | 2         |
| 1178     | .     | 200 | GLU  | HG2  | 2.331      | 0.02        | 2         |
| 1179     | .     | 200 | GLU  | HG3  | 2.404      | 0.02        | 2         |
| 1180     | .     | 200 | GLU  | CA   | 59.942     | 0.20        | 1         |
| 1181     | .     | 200 | GLU  | CB   | 28.896     | 0.20        | 1         |
| 1182     | .     | 200 | GLU  | CG   | 36.217     | 0.20        | 1         |
| 1183     | .     | 200 | GLU  | N    | 119.964    | 0.20        | 1         |
| 1184     | .     | 201 | THR  | H    | 7.913      | 0.02        | 1         |
| 1185     | .     | 201 | THR  | HA   | 3.795      | 0.02        | 1         |
| 1186     | .     | 201 | THR  | HB   | 3.705      | 0.02        | 1         |
| 1187     | .     | 201 | THR  | HG2  | 0.690      | 0.02        | 1         |
| 1188     | .     | 201 | THR  | HG2  | 0.690      | 0.02        | 1         |
| 1189     | .     | 201 | THR  | HG2  | 0.690      | 0.02        | 1         |
| 1190     | .     | 201 | THR  | CA   | 66.806     | 0.20        | 1         |
| 1191     | .     | 201 | THR  | CB   | 68.710     | 0.20        | 1         |
| 1192     | .     | 201 | THR  | CG2  | 21.070     | 0.20        | 1         |
| 1193     | .     | 201 | THR  | N    | 116.156    | 0.20        | 1         |
| 1194     | .     | 202 | ASP  | H    | 7.475      | 0.02        | 1         |
| 1195     | .     | 202 | ASP  | HA   | 4.585      | 0.02        | 1         |
| 1196     | .     | 202 | ASP  | HB2  | 3.346      | 0.02        | 2         |
| 1197     | .     | 202 | ASP  | HB3  | 2.634      | 0.02        | 2         |
| 1198     | .     | 202 | ASP  | CA   | 58.007     | 0.20        | 1         |
| 1199     | .     | 202 | ASP  | CB   | 41.647     | 0.20        | 1         |
| 1200     | .     | 202 | ASP  | N    | 120.044    | 0.20        | 1         |
| 1201     | .     | 203 | VAL  | H    | 8.187      | 0.02        | 1         |
| 1202     | .     | 203 | VAL  | HA   | 3.309      | 0.02        | 1         |
| 1203     | .     | 203 | VAL  | HB   | 2.101      | 0.02        | 1         |
| 1204     | .     | 203 | VAL  | HG1  | 0.979      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1205     | .     | 203 | VAL  | HG1  | 0.979      | 0.02        | 2         |
| 1206     | .     | 203 | VAL  | HG1  | 0.979      | 0.02        | 2         |
| 1207     | .     | 203 | VAL  | HG2  | 0.956      | 0.02        | 2         |
| 1208     | .     | 203 | VAL  | HG2  | 0.956      | 0.02        | 2         |
| 1209     | .     | 203 | VAL  | HG2  | 0.956      | 0.02        | 2         |
| 1210     | .     | 203 | VAL  | CA   | 67.786     | 0.20        | 1         |
| 1211     | .     | 203 | VAL  | CB   | 31.636     | 0.20        | 1         |
| 1212     | .     | 203 | VAL  | CG1  | 22.846     | 0.20        | 2         |
| 1213     | .     | 203 | VAL  | CG2  | 21.202     | 0.20        | 2         |
| 1214     | .     | 203 | VAL  | N    | 119.560    | 0.20        | 1         |
| 1215     | .     | 204 | LYS  | H    | 7.712      | 0.02        | 1         |
| 1216     | .     | 204 | LYS  | HA   | 4.079      | 0.02        | 1         |
| 1217     | .     | 204 | LYS  | HB2  | 1.966      | 0.02        | 2         |
| 1218     | .     | 204 | LYS  | HB3  | 1.900      | 0.02        | 2         |
| 1219     | .     | 204 | LYS  | HG2  | 1.450      | 0.02        | 2         |
| 1220     | .     | 204 | LYS  | HG3  | 1.502      | 0.02        | 2         |
| 1221     | .     | 204 | LYS  | HD2  | 1.665      | 0.02        | 2         |
| 1222     | .     | 204 | LYS  | HD3  | 1.665      | 0.02        | 2         |
| 1223     | .     | 204 | LYS  | HE2  | 2.965      | 0.02        | 2         |
| 1224     | .     | 204 | LYS  | HE3  | 2.905      | 0.02        | 2         |
| 1225     | .     | 204 | LYS  | CA   | 59.283     | 0.20        | 1         |
| 1226     | .     | 204 | LYS  | CB   | 32.133     | 0.20        | 1         |
| 1227     | .     | 204 | LYS  | CG   | 25.021     | 0.20        | 1         |
| 1228     | .     | 204 | LYS  | CD   | 29.053     | 0.20        | 1         |
| 1229     | .     | 204 | LYS  | CE   | 41.949     | 0.20        | 1         |
| 1230     | .     | 204 | LYS  | N    | 119.069    | 0.20        | 1         |
| 1231     | .     | 205 | MET  | H    | 8.156      | 0.02        | 1         |
| 1232     | .     | 205 | MET  | HA   | 4.165      | 0.02        | 1         |
| 1233     | .     | 205 | MET  | HB2  | 1.965      | 0.02        | 2         |
| 1234     | .     | 205 | MET  | HB3  | 2.153      | 0.02        | 2         |
| 1235     | .     | 205 | MET  | HG2  | 2.360      | 0.02        | 2         |
| 1236     | .     | 205 | MET  | HG3  | 2.929      | 0.02        | 2         |
| 1237     | .     | 205 | MET  | HE   | 1.491      | 0.02        | 1         |
| 1238     | .     | 205 | MET  | HE   | 1.491      | 0.02        | 1         |
| 1239     | .     | 205 | MET  | HE   | 1.491      | 0.02        | 1         |
| 1240     | .     | 205 | MET  | CA   | 60.021     | 0.20        | 1         |
| 1241     | .     | 205 | MET  | CB   | 32.775     | 0.20        | 1         |
| 1242     | .     | 205 | MET  | CG   | 34.124     | 0.20        | 1         |
| 1243     | .     | 205 | MET  | CE   | 18.249     | 0.20        | 1         |
| 1244     | .     | 205 | MET  | N    | 118.536    | 0.20        | 1         |
| 1245     | .     | 206 | MET  | H    | 8.715      | 0.02        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1246     | .     | 206 | MET  | HA   | 3.558      | 0.02        | 1         |
| 1247     | .     | 206 | MET  | HB2  | 2.148      | 0.02        | 2         |
| 1248     | .     | 206 | MET  | HB3  | 1.509      | 0.02        | 2         |
| 1249     | .     | 206 | MET  | HG2  | 1.626      | 0.02        | 2         |
| 1250     | .     | 206 | MET  | HG3  | 1.953      | 0.02        | 2         |
| 1251     | .     | 206 | MET  | HE   | 1.307      | 0.02        | 1         |
| 1252     | .     | 206 | MET  | HE   | 1.307      | 0.02        | 1         |
| 1253     | .     | 206 | MET  | HE   | 1.307      | 0.02        | 1         |
| 1254     | .     | 206 | MET  | CA   | 59.987     | 0.20        | 1         |
| 1255     | .     | 206 | MET  | CB   | 33.418     | 0.20        | 1         |
| 1256     | .     | 206 | MET  | CG   | 33.136     | 0.20        | 1         |
| 1257     | .     | 206 | MET  | CE   | 15.993     | 0.20        | 1         |
| 1258     | .     | 206 | MET  | N    | 118.192    | 0.20        | 1         |
| 1259     | .     | 207 | GLU  | H    | 8.445      | 0.02        | 1         |
| 1260     | .     | 207 | GLU  | HA   | 3.662      | 0.02        | 1         |
| 1261     | .     | 207 | GLU  | HB2  | 2.059      | 0.02        | 2         |
| 1262     | .     | 207 | GLU  | HB3  | 2.132      | 0.02        | 2         |
| 1263     | .     | 207 | GLU  | HG2  | 2.525      | 0.02        | 2         |
| 1264     | .     | 207 | GLU  | HG3  | 2.525      | 0.02        | 2         |
| 1265     | .     | 207 | GLU  | CA   | 60.789     | 0.20        | 1         |
| 1266     | .     | 207 | GLU  | CB   | 29.026     | 0.20        | 1         |
| 1267     | .     | 207 | GLU  | CG   | 35.996     | 0.20        | 1         |
| 1268     | .     | 207 | GLU  | N    | 118.792    | 0.20        | 1         |
| 1269     | .     | 208 | ARG  | H    | 7.240      | 0.02        | 1         |
| 1270     | .     | 208 | ARG  | HA   | 4.216      | 0.02        | 1         |
| 1271     | .     | 208 | ARG  | HB2  | 1.953      | 0.02        | 2         |
| 1272     | .     | 208 | ARG  | HB3  | 2.076      | 0.02        | 2         |
| 1273     | .     | 208 | ARG  | HG2  | 1.841      | 0.02        | 2         |
| 1274     | .     | 208 | ARG  | HG3  | 1.761      | 0.02        | 2         |
| 1275     | .     | 208 | ARG  | HD2  | 3.158      | 0.02        | 2         |
| 1276     | .     | 208 | ARG  | HD3  | 3.254      | 0.02        | 2         |
| 1277     | .     | 208 | ARG  | CA   | 58.463     | 0.20        | 1         |
| 1278     | .     | 208 | ARG  | CB   | 30.010     | 0.20        | 1         |
| 1279     | .     | 208 | ARG  | CG   | 26.943     | 0.20        | 1         |
| 1280     | .     | 208 | ARG  | CD   | 42.636     | 0.20        | 1         |
| 1281     | .     | 208 | ARG  | N    | 116.617    | 0.20        | 1         |
| 1282     | .     | 209 | VAL  | H    | 8.249      | 0.02        | 1         |
| 1283     | .     | 209 | VAL  | HA   | 3.775      | 0.02        | 1         |
| 1284     | .     | 209 | VAL  | HB   | 1.891      | 0.02        | 1         |
| 1285     | .     | 209 | VAL  | HG1  | 1.313      | 0.02        | 2         |
| 1286     | .     | 209 | VAL  | HG1  | 1.313      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1287     | .     | 209 | VAL  | HG1  | 1.313      | 0.02        | 2         |
| 1288     | .     | 209 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 1289     | .     | 209 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 1290     | .     | 209 | VAL  | HG2  | 0.957      | 0.02        | 2         |
| 1291     | .     | 209 | VAL  | CA   | 66.071     | 0.20        | 1         |
| 1292     | .     | 209 | VAL  | CB   | 32.287     | 0.20        | 1         |
| 1293     | .     | 209 | VAL  | CG1  | 24.119     | 0.20        | 2         |
| 1294     | .     | 209 | VAL  | CG2  | 21.152     | 0.20        | 2         |
| 1295     | .     | 209 | VAL  | N    | 119.315    | 0.20        | 1         |
| 1296     | .     | 210 | ILE  | H    | 9.037      | 0.02        | 1         |
| 1297     | .     | 210 | ILE  | HA   | 3.689      | 0.02        | 1         |
| 1298     | .     | 210 | ILE  | HB   | 2.015      | 0.02        | 1         |
| 1299     | .     | 210 | ILE  | HG12 | 1.747      | 0.02        | 2         |
| 1300     | .     | 210 | ILE  | HG13 | 0.961      | 0.02        | 2         |
| 1301     | .     | 210 | ILE  | HG2  | 1.189      | 0.02        | 1         |
| 1302     | .     | 210 | ILE  | HG2  | 1.189      | 0.02        | 1         |
| 1303     | .     | 210 | ILE  | HG2  | 1.189      | 0.02        | 1         |
| 1304     | .     | 210 | ILE  | HD1  | 0.723      | 0.02        | 1         |
| 1305     | .     | 210 | ILE  | HD1  | 0.723      | 0.02        | 1         |
| 1306     | .     | 210 | ILE  | HD1  | 0.723      | 0.02        | 1         |
| 1307     | .     | 210 | ILE  | CA   | 64.847     | 0.20        | 1         |
| 1308     | .     | 210 | ILE  | CB   | 37.104     | 0.20        | 1         |
| 1309     | .     | 210 | ILE  | CG1  | 30.122     | 0.20        | 1         |
| 1310     | .     | 210 | ILE  | CG2  | 20.624     | 0.20        | 1         |
| 1311     | .     | 210 | ILE  | CD1  | 14.471     | 0.20        | 1         |
| 1312     | .     | 210 | ILE  | N    | 121.172    | 0.20        | 1         |
| 1313     | .     | 211 | GLU  | H    | 7.975      | 0.02        | 1         |
| 1314     | .     | 211 | GLU  | HA   | 3.590      | 0.02        | 1         |
| 1315     | .     | 211 | GLU  | HB2  | 2.063      | 0.02        | 2         |
| 1316     | .     | 211 | GLU  | HB3  | 2.168      | 0.02        | 2         |
| 1317     | .     | 211 | GLU  | HG2  | 2.143      | 0.02        | 2         |
| 1318     | .     | 211 | GLU  | HG3  | 2.088      | 0.02        | 2         |
| 1319     | .     | 211 | GLU  | CA   | 61.193     | 0.20        | 1         |
| 1320     | .     | 211 | GLU  | CB   | 29.283     | 0.20        | 1         |
| 1321     | .     | 211 | GLU  | CG   | 36.053     | 0.20        | 1         |
| 1322     | .     | 211 | GLU  | N    | 120.604    | 0.20        | 1         |
| 1323     | .     | 212 | GLN  | H    | 7.147      | 0.02        | 1         |
| 1324     | .     | 212 | GLN  | HA   | 3.690      | 0.02        | 1         |
| 1325     | .     | 212 | GLN  | HB2  | 2.113      | 0.02        | 2         |
| 1326     | .     | 212 | GLN  | HB3  | 2.113      | 0.02        | 2         |
| 1327     | .     | 212 | GLN  | HG2  | 2.392      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1328     | .     | 212 | GLN  | HG3  | 2.452      | 0.02        | 2         |
| 1329     | .     | 212 | GLN  | HE21 | 6.870      | 0.02        | 2         |
| 1330     | .     | 212 | GLN  | HE22 | 7.559      | 0.02        | 2         |
| 1331     | .     | 212 | GLN  | CA   | 58.882     | 0.20        | 1         |
| 1332     | .     | 212 | GLN  | CB   | 28.236     | 0.20        | 1         |
| 1333     | .     | 212 | GLN  | CG   | 33.806     | 0.20        | 1         |
| 1334     | .     | 212 | GLN  | N    | 114.684    | 0.20        | 1         |
| 1335     | .     | 212 | GLN  | NE2  | 113.391    | 0.20        | 1         |
| 1336     | .     | 213 | MET  | H    | 8.199      | 0.02        | 1         |
| 1337     | .     | 213 | MET  | HA   | 4.166      | 0.02        | 1         |
| 1338     | .     | 213 | MET  | HB2  | 1.969      | 0.02        | 2         |
| 1339     | .     | 213 | MET  | HB3  | 2.072      | 0.02        | 2         |
| 1340     | .     | 213 | MET  | HG2  | 2.212      | 0.02        | 2         |
| 1341     | .     | 213 | MET  | HG3  | 2.284      | 0.02        | 2         |
| 1342     | .     | 213 | MET  | HE   | 1.885      | 0.02        | 1         |
| 1343     | .     | 213 | MET  | HE   | 1.885      | 0.02        | 1         |
| 1344     | .     | 213 | MET  | HE   | 1.885      | 0.02        | 1         |
| 1345     | .     | 213 | MET  | CA   | 59.969     | 0.20        | 1         |
| 1346     | .     | 213 | MET  | CB   | 32.501     | 0.20        | 1         |
| 1347     | .     | 213 | MET  | CG   | 32.212     | 0.20        | 1         |
| 1348     | .     | 213 | MET  | CE   | 16.578     | 0.20        | 1         |
| 1349     | .     | 213 | MET  | N    | 119.536    | 0.20        | 1         |
| 1350     | .     | 214 | CYS  | H    | 9.255      | 0.02        | 1         |
| 1351     | .     | 214 | CYS  | HA   | 4.416      | 0.02        | 1         |
| 1352     | .     | 214 | CYS  | HB2  | 3.542      | 0.02        | 2         |
| 1353     | .     | 214 | CYS  | HB3  | 2.905      | 0.02        | 2         |
| 1354     | .     | 214 | CYS  | CA   | 59.938     | 0.20        | 1         |
| 1355     | .     | 214 | CYS  | CB   | 41.908     | 0.20        | 1         |
| 1356     | .     | 214 | CYS  | N    | 119.433    | 0.20        | 1         |
| 1357     | .     | 215 | ILE  | H    | 8.275      | 0.02        | 1         |
| 1358     | .     | 215 | ILE  | HA   | 3.579      | 0.02        | 1         |
| 1359     | .     | 215 | ILE  | HB   | 2.034      | 0.02        | 1         |
| 1360     | .     | 215 | ILE  | HG12 | 1.025      | 0.02        | 2         |
| 1361     | .     | 215 | ILE  | HG13 | 1.047      | 0.02        | 2         |
| 1362     | .     | 215 | ILE  | HG2  | 0.897      | 0.02        | 1         |
| 1363     | .     | 215 | ILE  | HG2  | 0.897      | 0.02        | 1         |
| 1364     | .     | 215 | ILE  | HG2  | 0.897      | 0.02        | 1         |
| 1365     | .     | 215 | ILE  | HD1  | 0.845      | 0.02        | 1         |
| 1366     | .     | 215 | ILE  | HD1  | 0.845      | 0.02        | 1         |
| 1367     | .     | 215 | ILE  | HD1  | 0.845      | 0.02        | 1         |
| 1368     | .     | 215 | ILE  | CA   | 66.796     | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1369     | .     | 215 | ILE  | CB   | 38.144     | 0.20        | 1         |
| 1370     | .     | 215 | ILE  | CG1  | 30.750     | 0.20        | 1         |
| 1371     | .     | 215 | ILE  | CG2  | 17.243     | 0.20        | 1         |
| 1372     | .     | 215 | ILE  | CD1  | 14.086     | 0.20        | 1         |
| 1373     | .     | 215 | ILE  | N    | 123.918    | 0.20        | 1         |
| 1374     | .     | 216 | THR  | H    | 8.071      | 0.02        | 1         |
| 1375     | .     | 216 | THR  | HA   | 3.964      | 0.02        | 1         |
| 1376     | .     | 216 | THR  | HB   | 4.319      | 0.02        | 1         |
| 1377     | .     | 216 | THR  | HG2  | 1.238      | 0.02        | 1         |
| 1378     | .     | 216 | THR  | HG2  | 1.238      | 0.02        | 1         |
| 1379     | .     | 216 | THR  | HG2  | 1.238      | 0.02        | 1         |
| 1380     | .     | 216 | THR  | CA   | 67.181     | 0.20        | 1         |
| 1381     | .     | 216 | THR  | CB   | 68.259     | 0.20        | 1         |
| 1382     | .     | 216 | THR  | CG2  | 21.453     | 0.20        | 1         |
| 1383     | .     | 216 | THR  | N    | 118.680    | 0.20        | 1         |
| 1384     | .     | 217 | GLN  | H    | 8.735      | 0.02        | 1         |
| 1385     | .     | 217 | GLN  | HA   | 3.638      | 0.02        | 1         |
| 1386     | .     | 217 | GLN  | HB2  | 2.095      | 0.02        | 2         |
| 1387     | .     | 217 | GLN  | HB3  | 2.127      | 0.02        | 2         |
| 1388     | .     | 217 | GLN  | HG2  | 2.282      | 0.02        | 2         |
| 1389     | .     | 217 | GLN  | HG3  | 2.346      | 0.02        | 2         |
| 1390     | .     | 217 | GLN  | HE21 | 7.269      | 0.02        | 2         |
| 1391     | .     | 217 | GLN  | HE22 | 6.865      | 0.02        | 2         |
| 1392     | .     | 217 | GLN  | CA   | 58.731     | 0.20        | 1         |
| 1393     | .     | 217 | GLN  | CB   | 28.256     | 0.20        | 1         |
| 1394     | .     | 217 | GLN  | CG   | 32.655     | 0.20        | 1         |
| 1395     | .     | 217 | GLN  | N    | 122.294    | 0.20        | 1         |
| 1396     | .     | 217 | GLN  | NE2  | 115.906    | 0.20        | 1         |
| 1397     | .     | 218 | TYR  | H    | 8.572      | 0.02        | 1         |
| 1398     | .     | 218 | TYR  | HA   | 2.965      | 0.02        | 1         |
| 1399     | .     | 218 | TYR  | HB2  | 3.118      | 0.02        | 2         |
| 1400     | .     | 218 | TYR  | HB3  | 2.747      | 0.02        | 2         |
| 1401     | .     | 218 | TYR  | HD1  | 6.239      | 0.02        | 3         |
| 1402     | .     | 218 | TYR  | HD2  | 6.239      | 0.02        | 3         |
| 1403     | .     | 218 | TYR  | HE1  | 6.553      | 0.02        | 3         |
| 1404     | .     | 218 | TYR  | HE2  | 6.553      | 0.02        | 3         |
| 1405     | .     | 218 | TYR  | CA   | 62.140     | 0.20        | 1         |
| 1406     | .     | 218 | TYR  | CB   | 37.090     | 0.20        | 1         |
| 1407     | .     | 218 | TYR  | CD1  | 132.610    | 0.20        | 3         |
| 1408     | .     | 218 | TYR  | CD2  | 132.610    | 0.20        | 3         |
| 1409     | .     | 218 | TYR  | CE1  | 117.785    | 0.20        | 3         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1410     | .     | 218 | TYR  | CE2  | 117.785    | 0.20        | 3         |
| 1411     | .     | 218 | TYR  | N    | 121.449    | 0.20        | 1         |
| 1412     | .     | 219 | GLU  | H    | 8.263      | 0.02        | 1         |
| 1413     | .     | 219 | GLU  | HA   | 3.708      | 0.02        | 1         |
| 1414     | .     | 219 | GLU  | HB2  | 2.350      | 0.02        | 2         |
| 1415     | .     | 219 | GLU  | HB3  | 2.056      | 0.02        | 2         |
| 1416     | .     | 219 | GLU  | HG2  | 2.330      | 0.02        | 2         |
| 1417     | .     | 219 | GLU  | HG3  | 2.602      | 0.02        | 2         |
| 1418     | .     | 219 | GLU  | CA   | 59.798     | 0.20        | 1         |
| 1419     | .     | 219 | GLU  | CB   | 28.667     | 0.20        | 1         |
| 1420     | .     | 219 | GLU  | CG   | 35.781     | 0.20        | 1         |
| 1421     | .     | 219 | GLU  | N    | 121.232    | 0.20        | 1         |
| 1422     | .     | 220 | ARG  | H    | 7.908      | 0.02        | 1         |
| 1423     | .     | 220 | ARG  | HA   | 3.980      | 0.02        | 1         |
| 1424     | .     | 220 | ARG  | HB2  | 1.832      | 0.02        | 2         |
| 1425     | .     | 220 | ARG  | HB3  | 1.803      | 0.02        | 2         |
| 1426     | .     | 220 | ARG  | HG2  | 1.618      | 0.02        | 2         |
| 1427     | .     | 220 | ARG  | HG3  | 1.618      | 0.02        | 2         |
| 1428     | .     | 220 | ARG  | HD2  | 2.914      | 0.02        | 2         |
| 1429     | .     | 220 | ARG  | HD3  | 2.882      | 0.02        | 2         |
| 1430     | .     | 220 | ARG  | CA   | 59.240     | 0.20        | 1         |
| 1431     | .     | 220 | ARG  | CB   | 30.659     | 0.20        | 1         |
| 1432     | .     | 220 | ARG  | CG   | 27.195     | 0.20        | 1         |
| 1433     | .     | 220 | ARG  | CD   | 43.293     | 0.20        | 1         |
| 1434     | .     | 220 | ARG  | N    | 119.081    | 0.20        | 1         |
| 1435     | .     | 221 | GLU  | H    | 8.440      | 0.02        | 1         |
| 1436     | .     | 221 | GLU  | HA   | 4.023      | 0.02        | 1         |
| 1437     | .     | 221 | GLU  | HB2  | 2.157      | 0.02        | 2         |
| 1438     | .     | 221 | GLU  | HB3  | 1.952      | 0.02        | 2         |
| 1439     | .     | 221 | GLU  | HG2  | 2.417      | 0.02        | 2         |
| 1440     | .     | 221 | GLU  | HG3  | 2.200      | 0.02        | 2         |
| 1441     | .     | 221 | GLU  | CA   | 57.895     | 0.20        | 1         |
| 1442     | .     | 221 | GLU  | CB   | 29.090     | 0.20        | 1         |
| 1443     | .     | 221 | GLU  | CG   | 36.600     | 0.20        | 1         |
| 1444     | .     | 221 | GLU  | N    | 119.257    | 0.20        | 1         |
| 1445     | .     | 222 | SER  | H    | 8.458      | 0.02        | 1         |
| 1446     | .     | 222 | SER  | HA   | 3.896      | 0.02        | 1         |
| 1447     | .     | 222 | SER  | HB2  | 3.607      | 0.02        | 2         |
| 1448     | .     | 222 | SER  | HB3  | 3.381      | 0.02        | 2         |
| 1449     | .     | 222 | SER  | CA   | 61.378     | 0.20        | 1         |
| 1450     | .     | 222 | SER  | CB   | 62.508     | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1451     | .     | 222 | SER  | N    | 115.812    | 0.20        | 1         |
| 1452     | .     | 223 | GLN  | H    | 7.586      | 0.02        | 1         |
| 1453     | .     | 223 | GLN  | HA   | 4.116      | 0.02        | 1         |
| 1454     | .     | 223 | GLN  | HB2  | 2.110      | 0.02        | 2         |
| 1455     | .     | 223 | GLN  | HB3  | 2.110      | 0.02        | 2         |
| 1456     | .     | 223 | GLN  | HG2  | 2.361      | 0.02        | 2         |
| 1457     | .     | 223 | GLN  | HG3  | 2.500      | 0.02        | 2         |
| 1458     | .     | 223 | GLN  | HE21 | 7.471      | 0.02        | 2         |
| 1459     | .     | 223 | GLN  | HE22 | 6.783      | 0.02        | 2         |
| 1460     | .     | 223 | GLN  | CA   | 58.305     | 0.20        | 1         |
| 1461     | .     | 223 | GLN  | CB   | 28.281     | 0.20        | 1         |
| 1462     | .     | 223 | GLN  | CG   | 33.937     | 0.20        | 1         |
| 1463     | .     | 223 | GLN  | N    | 120.340    | 0.20        | 1         |
| 1464     | .     | 223 | GLN  | NE2  | 111.759    | 0.20        | 1         |
| 1465     | .     | 224 | ALA  | H    | 7.486      | 0.02        | 1         |
| 1466     | .     | 224 | ALA  | HA   | 4.168      | 0.02        | 1         |
| 1467     | .     | 224 | ALA  | HB   | 1.416      | 0.02        | 1         |
| 1468     | .     | 224 | ALA  | HB   | 1.416      | 0.02        | 1         |
| 1469     | .     | 224 | ALA  | HB   | 1.416      | 0.02        | 1         |
| 1470     | .     | 224 | ALA  | CA   | 54.095     | 0.20        | 1         |
| 1471     | .     | 224 | ALA  | CB   | 18.501     | 0.20        | 1         |
| 1472     | .     | 224 | ALA  | N    | 120.710    | 0.20        | 1         |
| 1473     | .     | 225 | TYR  | HD1  | 6.667      | 0.02        | 3         |
| 1474     | .     | 225 | TYR  | HD2  | 6.667      | 0.02        | 3         |
| 1475     | .     | 225 | TYR  | CD1  | 133.135    | 0.20        | 3         |
| 1476     | .     | 225 | TYR  | CD2  | 133.135    | 0.20        | 3         |
| 1477     | .     | 226 | TYR  | H    | 7.962      | 0.02        | 1         |
| 1478     | .     | 226 | TYR  | HA   | 4.361      | 0.02        | 1         |
| 1479     | .     | 226 | TYR  | HB2  | 3.163      | 0.02        | 2         |
| 1480     | .     | 226 | TYR  | HB3  | 2.933      | 0.02        | 2         |
| 1481     | .     | 226 | TYR  | HD1  | 7.205      | 0.02        | 3         |
| 1482     | .     | 226 | TYR  | HD2  | 7.205      | 0.02        | 3         |
| 1483     | .     | 226 | TYR  | HE1  | 7.095      | 0.02        | 3         |
| 1484     | .     | 226 | TYR  | HE2  | 7.095      | 0.02        | 3         |
| 1485     | .     | 226 | TYR  | CA   | 59.353     | 0.20        | 1         |
| 1486     | .     | 226 | TYR  | CB   | 38.091     | 0.20        | 1         |
| 1487     | .     | 226 | TYR  | CD1  | 133.321    | 0.20        | 3         |
| 1488     | .     | 226 | TYR  | CD2  | 133.321    | 0.20        | 3         |
| 1489     | .     | 226 | TYR  | CE1  | 118.314    | 0.20        | 3         |
| 1490     | .     | 226 | TYR  | CE2  | 118.314    | 0.20        | 3         |
| 1491     | .     | 226 | TYR  | N    | 117.916    | 0.20        | 1         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1492     | .     | 227 | GLN  | H    | 7.845      | 0.02        | 1         |
| 1493     | .     | 227 | GLN  | HA   | 4.233      | 0.02        | 1         |
| 1494     | .     | 227 | GLN  | HB2  | 2.057      | 0.02        | 2         |
| 1495     | .     | 227 | GLN  | HB3  | 2.140      | 0.02        | 2         |
| 1496     | .     | 227 | GLN  | HG2  | 2.403      | 0.02        | 2         |
| 1497     | .     | 227 | GLN  | HG3  | 2.331      | 0.02        | 2         |
| 1498     | .     | 227 | GLN  | HE21 | 7.449      | 0.02        | 2         |
| 1499     | .     | 227 | GLN  | HE22 | 6.806      | 0.02        | 2         |
| 1500     | .     | 227 | GLN  | CA   | 56.481     | 0.20        | 1         |
| 1501     | .     | 227 | GLN  | CB   | 28.830     | 0.20        | 1         |
| 1502     | .     | 227 | GLN  | CG   | 33.989     | 0.20        | 1         |
| 1503     | .     | 227 | GLN  | N    | 119.353    | 0.20        | 1         |
| 1504     | .     | 227 | GLN  | NE2  | 111.904    | 0.20        | 1         |
| 1505     | .     | 228 | ARG  | H    | 7.916      | 0.02        | 1         |
| 1506     | .     | 228 | ARG  | HA   | 4.210      | 0.02        | 1         |
| 1507     | .     | 228 | ARG  | HB2  | 1.817      | 0.02        | 2         |
| 1508     | .     | 228 | ARG  | HB3  | 1.817      | 0.02        | 2         |
| 1509     | .     | 228 | ARG  | HG2  | 1.616      | 0.02        | 2         |
| 1510     | .     | 228 | ARG  | HG3  | 1.687      | 0.02        | 2         |
| 1511     | .     | 228 | ARG  | HD2  | 3.207      | 0.02        | 2         |
| 1512     | .     | 228 | ARG  | HD3  | 3.128      | 0.02        | 2         |
| 1513     | .     | 228 | ARG  | CA   | 56.870     | 0.20        | 1         |
| 1514     | .     | 228 | ARG  | CB   | 30.698     | 0.20        | 1         |
| 1515     | .     | 228 | ARG  | CG   | 27.224     | 0.20        | 1         |
| 1516     | .     | 228 | ARG  | CD   | 43.569     | 0.20        | 1         |
| 1517     | .     | 228 | ARG  | N    | 120.687    | 0.20        | 1         |
| 1518     | .     | 229 | GLY  | H    | 8.225      | 0.02        | 1         |
| 1519     | .     | 229 | GLY  | HA2  | 3.979      | 0.02        | 2         |
| 1520     | .     | 229 | GLY  | HA3  | 3.979      | 0.02        | 2         |
| 1521     | .     | 229 | GLY  | CA   | 45.379     | 0.20        | 1         |
| 1522     | .     | 229 | GLY  | N    | 109.167    | 0.20        | 1         |
| 1523     | .     | 230 | SER  | H    | 8.111      | 0.02        | 1         |
| 1524     | .     | 230 | SER  | HA   | 4.492      | 0.02        | 1         |
| 1525     | .     | 230 | SER  | HB2  | 3.870      | 0.02        | 2         |
| 1526     | .     | 230 | SER  | HB3  | 3.870      | 0.02        | 2         |
| 1527     | .     | 230 | SER  | CA   | 58.266     | 0.20        | 1         |
| 1528     | .     | 230 | SER  | CB   | 64.051     | 0.20        | 1         |
| 1529     | .     | 230 | SER  | N    | 115.696    | 0.20        | 1         |
| 1530     | .     | 231 | SER  | H    | 7.983      | 0.02        | 1         |
| 1531     | .     | 231 | SER  | HA   | 4.296      | 0.02        | 1         |
| 1532     | .     | 231 | SER  | HB2  | 3.856      | 0.02        | 2         |

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| Shift ID | Chain | Res | Type | Atom | Shift Data |             |           |
|----------|-------|-----|------|------|------------|-------------|-----------|
|          |       |     |      |      | Value      | Uncertainty | Ambiguity |
| 1533     | .     | 231 | SER  | HB3  | 3.856      | 0.02        | 2         |
| 1534     | .     | 231 | SER  | CA   | 60.086     | 0.20        | 1         |
| 1535     | .     | 231 | SER  | CB   | 64.840     | 0.20        | 1         |
| 1536     | .     | 231 | SER  | N    | 122.862    | 0.20        | 1         |

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

No chemical shift referencing corrections were calculated (not enough data).

### 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1224. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total       | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-------------|----------------|-----------------|-----------------|
| Backbone  | 0/484 (0%)  | 0/193 (0%)     | 0/196 (0%)      | 0/95 (0%)       |
| Sidechain | 0/621 (0%)  | 0/365 (0%)     | 0/221 (0%)      | 0/35 (0%)       |
| Aromatic  | 0/119 (0%)  | 0/63 (0%)      | 0/52 (0%)       | 0/4 (0%)        |
| Overall   | 0/1224 (0%) | 0/621 (0%)     | 0/469 (0%)      | 0/134 (0%)      |

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1779. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|           | Total       | <sup>1</sup> H | <sup>13</sup> C | <sup>15</sup> N |
|-----------|-------------|----------------|-----------------|-----------------|
| Backbone  | 0/723 (0%)  | 0/288 (0%)     | 0/294 (0%)      | 0/141 (0%)      |
| Sidechain | 0/887 (0%)  | 0/527 (0%)     | 0/311 (0%)      | 0/49 (0%)       |
| Aromatic  | 0/169 (0%)  | 0/89 (0%)      | 0/73 (0%)       | 0/7 (0%)        |
| Overall   | 0/1779 (0%) | 0/904 (0%)     | 0/678 (0%)      | 0/197 (0%)      |

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

There are no statistically unusual chemical shifts.

### 7.1.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned\_chem\_shift\_list\_1). RCI is only applicable to proteins.