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Solution structure refinement comparing reference model NOE volumes

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SOLUTION STRUCTURE REFINEMENT COMPARING REFERENCE MODEL NOE VOLUMES

By

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ABSTRACT

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NMR is a powerful experimental technique which can be used to determine protein structures. Central to this process is conversion of peak volumes in the NOE data sets into distance constraints and then structural refinement against those constraints. In general, each solution structural analysis is initiated de novo. We are interested in the structural analysis of a series of hybrids derived from two parental proteins (rubredoxins from mesophilic bacterium *Clostridium pasteurianum* (*Cp*) and the hyperthermophilic archaeon *Pyrococcus furiosus* (*Pf*)). Near 1 Å resolution X-ray structures of *Cp* and *Pf* rubredoxins are available to provide a basis for quantitative comparison of the NOE volumes for analogous 1H-1H pairs in a difference analysis. In this approach, the volume differences are used to drive the structure away from the initial parentally derived model.

Introduction

Proteins are relatively large, complex molecules that are stable in solution only under certain specific conditions. The degree of stability depends greatly on the environment in which the protein is normally found. Environments that are extreme in temperature, pressure or pH cause most proteins to denature and/or decompose. However, thermophiles and hyperthermophiles constitute a group of proteins that defy the norm. Discovered in extreme temperature environments such as geothermal hot springs, they are stable enough to withstand extreme environments without denaturing or decomposing. Our goal is to explore these anomalous proteins and to investigate their unusually high stability through computer models, energy calculations, and nuclear magnetic resonance experiments.

Mesophilic, thermophilic and hyperthermophilic enzymes are all naturally-occurring; however, each type of enzyme differs significantly in thermal stability. Mesophilic enzymes, found in most living organisms, have an optimal growth temperature of 25°C to 50°C. Thermophilic enzymes, found in more extreme temperature environments than mesophiles, grow optimally between 50°C and 80°C. Hyperthermophilic enzymes, found in highly extreme temperature environments such as thermal hot springs or the ocean floor, are optimally active between 80°C and 110°C.[1]

There have been many hypotheses proposed that try to explain the unusual thermostability of thermophiles and hyperthermophiles. Several hypotheses include: van der Waals interactions between the β-strands, hydrogen bonding, and the presence of salt bridges within the molecule.[2] Another hypothesis relates rigidity to thermal stability. Thermophiles and hyperthermophiles are presumed to be relatively rigid molecules. This

rigid structure would help to explain the thermostability which allows thermophiles to withstand denaturation at temperatures up to 200°C. Mesophiles are believed to have more conformational flexibility which helps to explain why they rapidly denature at 80°C.[3]

The mesophile and thermophile used for this project are rubredoxins from *Clostridium pasteurianum* (*Cp*) and *Pyrococcus furiosus* (*Pf*), respectively. The amino acid sequences of *Cp* and *Pf* are listed in Figure 1.

```
Cp, 5RXN    MKKYTCTVCGYIYNPEDGDPDNGVNPGTDFKDIPDDWVCPLCGVGKDQFEEVEE
Pf, 1BQ8    MAKWVCKICGYIYDEDAGDPDNGISPGTKFEELPDDWVCPICGAPKSEFEKLED
```

Figure 1. Amino acid sequences of *Cp* (top) and *Pf* (bottom). The amino acids in black are where the two sequences are identical. The colored amino acids are where the two sequences differ from one another.

Cp and *Pf* are similar in size and absorption properties. Both proteins contain 54 residues and an iron metal center. Each Fe^{2+} is electrostatically bound to four cysteine molecules. Both proteins contain three α-helices, however, they differ in the number of β-strands. *Cp* contains four β-strands while *Pf* only contains three. The significant difference between the two lies within their thermostability.[4]

Cp and *Pf* are illustrated in Figure 2.

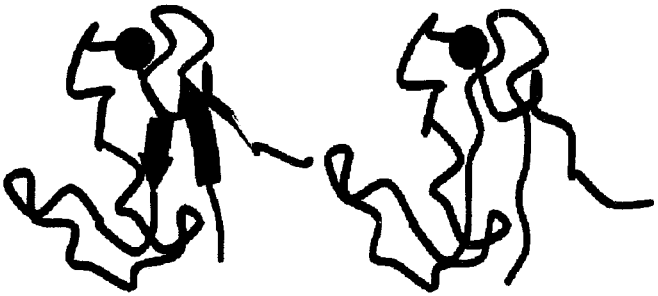


Figure 2. Figures created from Protein Data Bank crystal structures. *Cp* illustrated on left (5RXN[5]), *Pf* illustrated on right (1BQ8[6]). The broad arrows represent β-strands and each arrow points from the N terminus to the C terminus of the protein chain. The spheres represent the iron metal center. The rest of the figure illustrates that the other residues do not have any repeating secondary structure.

The purpose of this project was to model various hybrids using combinations of residues from *Cp* and *Pf* and to find the optimal geometry of each model. Hybrids of *Cp* and *Pf* were built to investigate and help determine the reason for the extreme thermostability of thermophiles and hyperthermophiles. The models were then used to calculate theoretical NOE peaks. The volumes of the calculated NOE peaks were compared to the experimentally-obtained NOE volumes. Discrepancies in peak volumes were used to modify the computer-generated models. Once all discrepancies had been removed, the models were assumed to accurately represent their corresponding hybrids.

The second aspect of this project was to write a computer program to automate the process of assigning protons from the structure to spectral NOE peaks. The program was designed to assign NOE peaks based on chemical shift information, while taking into account the uncertainty of the experimental measurements. In cases where more than one assignment was possible for a particular chemical shift, the program was designed to consult the corresponding computer model to determine which of the possible assignments was most likely. Therefore, the accurate models served, not only to illustrate hybrids for which no known crystal structures exist, but to be used as a reference for automating the lengthy, time-consuming process of assigning NOE peaks for these and other hybrids.

Methods

The first aspect of the project involved building accurate representations of the protein hybrids we wanted to model. Constructing the models involved several steps, including assigning partial charges to atoms, choosing an optimal force field to calculate the energy and optimize the geometry of the protein, setting parameters to best represent the coordination of the metal center, and choosing the most accurate way to construct hybrid proteins from the given crystal structures. This process of molecular modeling has been broken down into three main parts: molecular modeling, force field, and partial charges.

Molecular Modeling

All protein hybrids were constructed from two Protein Data Bank files, 5RXN[7] and 1BQ8[8]. All water molecules were removed from the original crystal structures and they were aligned using MidasPlus 2.1[9]. They were superimposed and matched along the backbone atoms (N,CA,C,O,HA) so that the starting structures of the hybrids had nearly identical backbones (RMSD of backbone atoms (N, O, C^{α}) for residues 1-53 between *Cp* and *Pf* was calculated to be 0.66Å). The sidechain starting conformations were selected from the aligned structures also. The resulting orientations were saved and used for hybridization.

Hydrogens and lone pairs of electrons were added to the protein hybrids using Macromodel. Macromodel was also used to fix D14N, D22N, and E48Q residues that had been incorrectly assigned in the crystal structure of *Cp* that was downloaded from the Protein Data Bank. Residues 14 and 22 were changed from ASP to ASN, and residue 48 was changed from GLU to GLN in *Cp*, and the iron metal center was replaced with zinc in both *Cp* and *Pf*. The ASN and GLN residues were incorrectly assigned as ASP or GLU because the electron density of nitrogen is close to that of oxygen, and the electron density of hydrogen is so small that all hydrogens are "invisible" in the X-ray experiment. Therefore, CH_2COO has about the same electron density as CH_2CONH_2, and the crystallographers had to guess. Macromodel was used to manually change the oxygen to a nitrogen and add a hydrogen for residues 14, 22 and 48. Energy minimizations were used to correct the geometry of the fixed residues.

The metal center was changed in the models to accurately reflect the change that was made experimentally. Since NMR was the instrument used for analysis, a diamagnetic

metal center (such as zinc) was needed to replace the naturally-occurring paramagnetic iron metal center. Both of the zinc metal centers were represented using the nonbonded approach (Zn···S(Cys) bonds were modeled with zero bond orders).

All semi-empirical and *ab initio* calculations were carried out using Spartan '02 Linux/Unix[13]. The model compound used was $[Zn(SCH_2CH_3)_4]^{2-}$. Geometry optimization was performed at the semi-empirical level using the AM1 model. The single point energy of that optimal structure was then calculated at the *ab initio* level using the 6-31G* density functional model.

Partial Charges

All subsequent modeling and computation was performed using Macromodel Interactive Molecular Modeling System Version 7.0[10]. Macromodel assigned partial charges to all the atoms in the protein as a result of energy calculations. The partial charges that Macromodel assigned to the backbone atoms were not changed to avoid altering torsion angles along the backbone. Equal amounts of charge were then distributed among the zinc and four cysteines, (the two lone pairs on each sulfur, CB, S, 1HB, and 2HB) to accurately model the charge on the four cysteines and the zinc metal center.

Force Field

Before the geometry of the hybrid was optimized, residue 2(LYS) was relaxed to minimize bad contacts with residue 1 and residue 3. The LYS residue was relaxed using two solvent shells. The first shell had a radius of 5.00 Å and a force constant of 200.00 kcal/mol $Å^2$. The second solvent shell had a radius of 8.00 Å and a force constant of 500.00 kcal/mol Å.

Geometry optimization was performed using the AMBER force field. Before using this force field, however, parameters for zinc were added because no such parameters existed for this program. Without parameters for zinc, the program could not perform any calculations, including those calculations involved in geometry optimization. The added parameters included: a zinc radius of 1.1Å, a well-depth of 0.0125 kcal, and a Zn-S bond length of 2.29Å with a force constant of 40 kcal/mol Å[11]. Also added were bond angles for C-S-Zn, H-S-Zn, and S-Zn-S. The values for these angles were obtained from the crystal structures of several rubredoxins in the Protein Data Bank. A force constant corresponding to each bond angle was also added. Those values were 20 kcal/mol · rad^2, 100 kcal/mol · rad^2, and 20 kcal/mol · rad^2 respectively[12].

Geometry optimization of the entire hybrid was accomplished via a constrained energy minimization using a well potential with a 0.1Å half-width. The backbone atoms were constrained with a force constant of 60 kcal/mol Å^2 and the sidechain atoms were constrained using a 30 kcal/mol Å^2 force constant. Geometry optimization was performed without a simulated water solvent.

Each hybrid was constructed using sections of each *Cp* and *Pf*. Since there are no existing crystal structures for any of these hybrids, there was no template to dictate the residue number at which each protein section should be cut. Therefore, multiple constructs of each hybrid were made. Each construct was geometrically optimized and the construct with the lowest total energy was chosen as the representative model for the corresponding hybrid. The lowest energy constructs were chosen as follows: the third of three BYRubredoxin constructs: *Pf* residues (1-11) + *Cp* residues (12-37) + *Pf* residues (38-54) – *Pf* residue (2) + *Cp* residue (2), the third of three RGRubredoxin constructs:

Cp(1-11) + *Pf*(12-37) + *Cp*(38-54), one YRubredoxin construct: *Pf*(1-5) + *Cp*(6-11) + *Pf*(12-37) + *Cp*(38-49) + *Pf*(50-54) - *Pf*(2) + *Cp*(2), and the second of two RGBRubredoxin constructs: *Pf*(1-5) + *Cp*(6-11) + *Pf*(12-37) + *Cp*(38-50) + *Pf*(51-54) – *Pf*(2) + *Cp*(2). The geometries of both crystal structures (*Cp* and A2K) were also optimized.

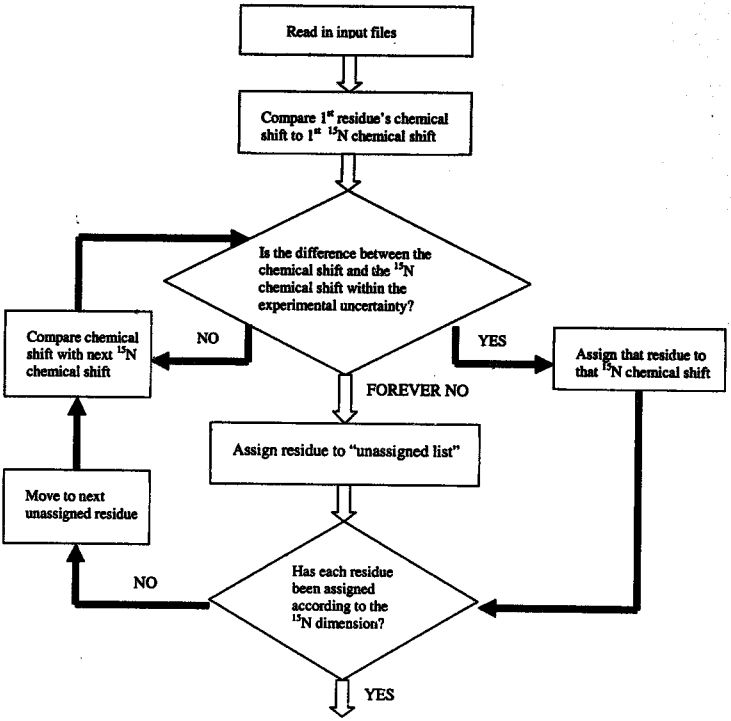
Purpose

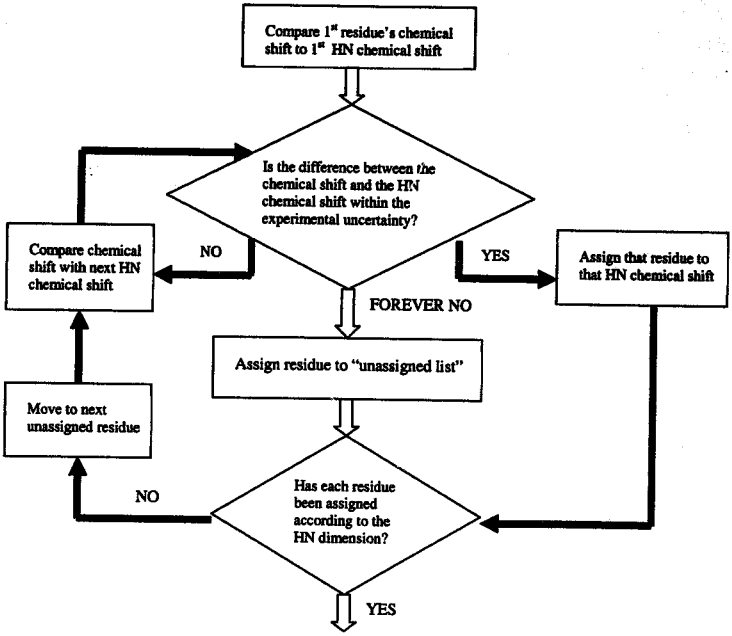
The purpose of this program is to automate the process of assigning protons to their respective NOE peaks. The input is three user-specified files: a file containing residue information (including residue names, residue numbers, and chemical shifts), a file containing NOE peak information (including peak volumes, and chemical shifts for the HN, HX and N^{15} dimensions), and a .pdb file containing the x, y, and z coordinates of each proton in the computer-generated model of the protein. Uncertainty values for each of the three NOE dimensions have been hard-coded into the program (const double D1_UNCERTAINTY, const double D2_UNCERTAINTY, and const double D3_UNCERTAINTY). The uncertainty values are based on spectral parameters (the experimental uncertainty in reading the NOE spectra), and should be changed accordingly with each new experiment. The output of this program is a tabulated text file containing unambiguously assigned, ambiguously assigned, and unassigned peaks, along with calculated distances between each set of peaks. All distances were calculated using the standard distance formula:

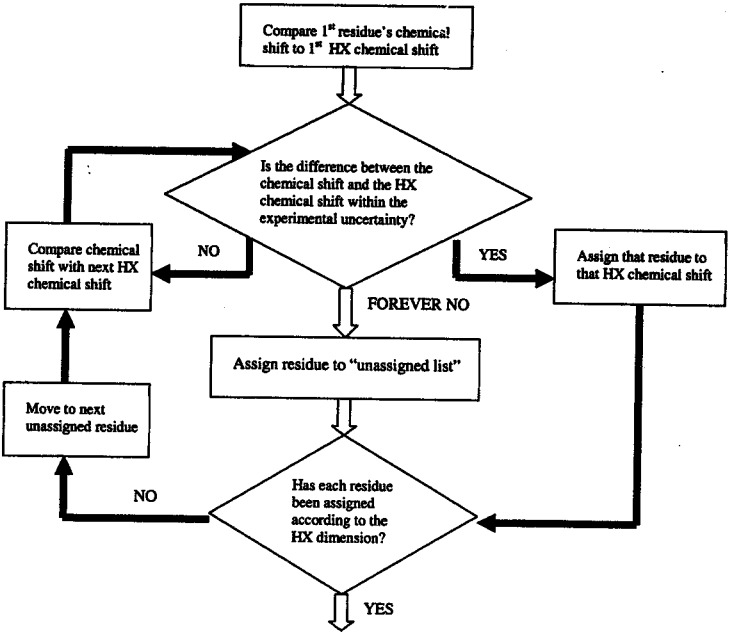
$d = SQRT[(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2]$.

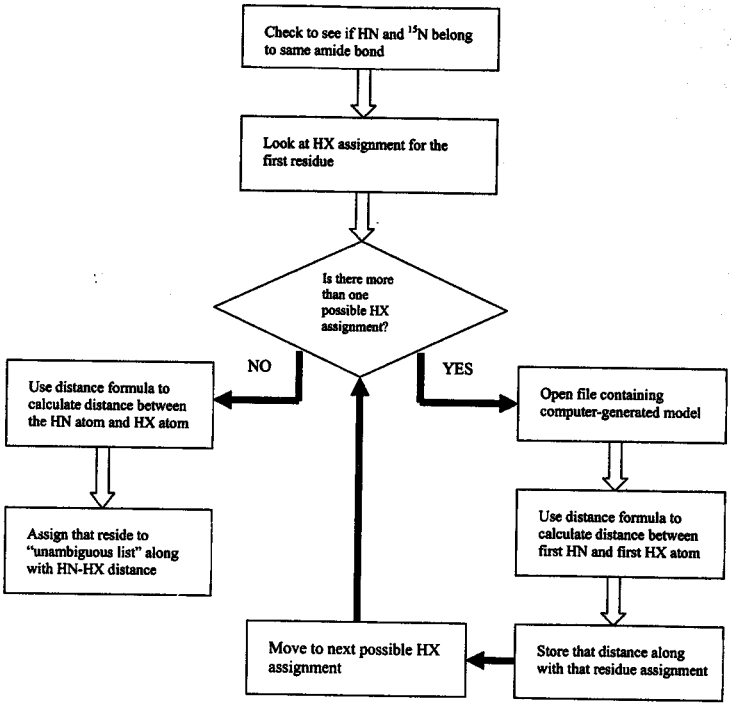
A flowchart illustrating the program protocol is listed below. The flowchart is a generalized step-by-step outline of the program. For further details, including specific functions and data structures used, see the source code following the flowchart.

Flow Chart


Read in input files
Compare 1st residue's chemical shift to 1st 15N chemical shift
Is the difference between the chemical shift and the 15N chemical shift within the experimental uncertainty?
NO
YES
Compare chemical shift with next 15N chemical shift
Assign that residue to that 15N chemical shift
FOREVER NO
Assign residue to "unassigned list"
Move to next unassigned residue
NO
Has each residue been assigned according to the 15N dimension?
YES


Compare 1st residue's chemical shift to 1st HN chemical shift
Is the difference between the chemical shift and the HN chemical shift within the experimental uncertainty?
NO
YES
Compare chemical shift with next HN chemical shift
Assign that residue to that HN chemical shift
FOREVER NO
Assign residue to "unassigned list"
Move to next unassigned residue
Has each residue been assigned according to the HN dimension?
NO
YES


Compare 1st residue's chemical shift to 1st HX chemical shift
Is the difference between the chemical shift and the HX chemical shift within the experimental uncertainty?
NO
YES
Compare chemical shift with next HX chemical shift
Assign that residue to that HX chemical shift
FOREVER NO
Assign residue to "unassigned list"
Move to next unassigned residue
NO
Has each residue been assigned according to the HX dimension?
YES


Check to see if HN and ^{15}N belong to same amide bond
Look at HX assignment for the first residue
Is there more than one possible HX assignment?
NO
YES
Use distance formula to calculate distance between the HN atom and HX atom
Assign that reside to "unambiguous list" along with HN-HX distance
Open file containing computer-generated model
Use distance formula to calculate distance between first HN and first HX atom
Store that distance along with that residue assignment
Move to next possible HX assignment

Source Code

```
/* Title:       NOE Program
 * Purpose:     READ IN TWO ARRAYS VIA USER-SPECIFIED FILE.
 *              MAKE RESIDUE ASSIGNMENTS USING 3D NOE PEAKS
 *              AND RESIDUE CHEMICAL SHIFTS
 * Written by: Maura Mahar
 * Date:        June 15, 2003
 ************************************************************************/

#include <iostream>                          // <<, >>, cin, cout
#include <fstream>                           //ifstream, ofstream
#include <cstdlib>                           //exit()
#include <iomanip>                           //setw() to format file output
#include <string>                            //load string library
#include <cmath>                             //abs, +, -, *, /


void print_help();

using namespace std;

int main(int argc,char *argv[])
{
time_t start_time;
time_t end_time;
start_time = time(NULL);

    if(argc > 1)
    {
        for(int y = 0; y < argc; y++)
        {
            if(argv[y][0] == '-' && argv[y][1] == 'h')
            {
                print_help();
                exit(0);
            }
        }
    }

int verbose = 0;

    if(argc > 1)
    {
        for(int y = 0; y < argc; y++)
        {
            if(argv[y][0] == '-' && argv[y][1] == 'v')
            {
                cout << "Running in verbose mode\n";
                verbose = 1;
            }
        }
    }
if(verbose == 1)
    {
    cout << "This program assigns NOE peaks based on ";
    cout << "chemical shifts and residue information" << endl;
    }
    ifstream ChemShift;                 //BYshifts, ordered file
    ifstream threeD_NOEInfo;            //BYRubactualNOES file
    ifstream proton_distances;          //.pdb file
    ofstream AssignedPeaks;             //output file

    int true_value = 0;
    const int NUM_ENTRIES = 10000;          //number of possible entries
    const int POSSIBLE_ASSIGNMENTS = 15;  //number of possible assignments
    const double D1_UNCERTAINTY = 0.018;  //uncertainty for HN dimension
    const double D2_UNCERTAINTY = 0.012;  //uncertainty for HX dimension
    const double D3_UNCERTAINTY = 0.375;  //uncertainty for 15N dimension
    int counts_d1[NUM_ENTRIES];
    int counts_d2[NUM_ENTRIES];
```

```
995       int counts_d3[NUM_ENTRIES];
996       int total_assigns_made = 0;
997
998       double Atom_Distance = 0.00;
999       double X1 = 0.00;
1000      double Y1 = 0.00;
1001      double Z1 = 0.00;
1002      double X2 = 0.00;
1003      double Y2 = 0.00;
1004      double Z2 = 0.00;                    //variables for distance formula
1005
1006
1007      int PeakNumber[NUM_ENTRIES];
1008      double ppm1[NUM_ENTRIES];
1009      double ppm2[NUM_ENTRIES];
1010      double ppm3[NUM_ENTRIES];            //arrays for 3D NOE file
1011
1012      string ResidueName[NUM_ENTRIES];
1013      int ResidueNumber[NUM_ENTRIES];
1014      string AtomName[NUM_ENTRIES];
1015      double ppm[NUM_ENTRIES];
1016      int order[NUM_ENTRIES];              //arrays for ChemShift file
1017
1018      double pdbX[NUM_ENTRIES];
1019      double pdbY[NUM_ENTRIES];
1020      double pdbZ[NUM_ENTRIES];
1021      string pdbAtm[NUM_ENTRIES];
1022      int pdbAtmNum[NUM_ENTRIES];
1023      string pdbAtmNam[NUM_ENTRIES];
1024      string pdbResNam[NUM_ENTRIES];
1025      int pdbResNum[NUM_ENTRIES];
1026      double pdbFoo[NUM_ENTRIES];
1027      double pdbBar[NUM_ENTRIES];
1028      double PeakVolume[NUM_ENTRIES];       //arrays for .pdb file
1029
1030      int Exp_Assign[NUM_ENTRIES];
1031
1032      char ChemShiftFile[30] = "ChemShift.txt";
1033      char proton_distances_file[30] = "pdbfile.txt";
1034      char AssignedPeaksFile[30] = "output.txt";
1035      char threeD_NOEInfoFile[30];
1036
1037
1038      double distances[NUM_ENTRIES][POSSIBLE_ASSIGNMENTS];
1039                           //array for calculated interproton distances
1040
1041
1042      int d1_assigns[NUM_ENTRIES][POSSIBLE_ASSIGNMENTS];
1043                           //array for residues assigned in D1 dimension
1044
1045  for(int i = 0; i < NUM_ENTRIES; i++)
1046      {
1047      for(int j = 0; j < POSSIBLE_ASSIGNMENTS; j++)
1048          {
1049          d1_assigns[i][j] = -5;
1050          }                    //initialize all values in array to -5
1051      }
1052      int D1_matches = 0;                   //number of D1 assignments
1053
1054      int d2_assigns[NUM_ENTRIES][POSSIBLE_ASSIGNMENTS];
1055                           //array for residues assigned in D2 dimension
1056
1057  for(int i = 0; i < NUM_ENTRIES; i++)
1058      {
1059      for(int j = 0; j < POSSIBLE_ASSIGNMENTS; j++)
1060          {
1061          d2_assigns[i][j] = -5;
1062          }                    //initialize all values in array to -5
1063      }
1064      int D2_matches = 0;                   //number of D2 assignments
1065
```

```
1066      int d3_assigns[NUM_ENTRIES][POSSIBLE_ASSIGNMENTS];
1067                          //array for residues assigned in D3 dimension
1068
1069  for(int i = 0; i < NUM_ENTRIES; i++)
1070      {
1071      for(int j = 0; j < POSSIBLE_ASSIGNMENTS; j++)
1072          {
1073          d3_assigns[i][j] = -5;
1074          }                   //initialize all values in array to -5
1075      }
1076
1077      int D3_matches = 0;                 //number of D3 assignments
1078
1079      int d1_reverse_assigns[NUM_ENTRIES][POSSIBLE_ASSIGNMENTS];
1080      for(int i = 0; i < NUM_ENTRIES; i++)
1081      {
1082          for(int j = 0; j < POSSIBLE_ASSIGNMENTS; j++)
1083          {
1084              d1_reverse_assigns[i][j] = -5;
1085          }
1086      }
1087
1088      int d2_reverse_assigns[NUM_ENTRIES][POSSIBLE_ASSIGNMENTS];
1089  for(int i = 0; i < NUM_ENTRIES; i++)
1090      {
1091          for(int j = 0; j < POSSIBLE_ASSIGNMENTS; j++)
1092          {
1093              d2_reverse_assigns[i][j] = -5;
1094          }
1095      }
1096
1097      int d3_reverse_assigns[NUM_ENTRIES][POSSIBLE_ASSIGNMENTS];
1098  for(int i = 0; i < NUM_ENTRIES; i++)
1099      {
1100          for(int j = 0; j < POSSIBLE_ASSIGNMENTS; j++)
1101          {
1102              d3_reverse_assigns[i][j] = -5;
1103          }
1104      }
1105
1106
1107
1108  if(argc == 1)
1109      {
1110          cout << "Please enter the name of the file containing";
1111          cout << " 3D NOE peak information: ";
1112
1113          cin >> threeD_NOEInfoFile;
1114          threeD_NOEInfo.open(threeD_NOEInfoFile);
1115          if(threeD_NOEInfo.fail())               //if file does not open
1116          {                                       //inform the user
1117              cout << "The input file could not be opened.\n";
1118              exit(1);                            //exit the program
1119          }
1120
1121          cout << "Please enter the name of the chemical shift file: ";
1122
1123          cin >> ChemShiftFile;
1124          ChemShift.open(ChemShiftFile);
1125          if(ChemShift.fail())                    //if file does not open
1126          {                                       //inform the user
1127              cout << "The input file could not be opened.\n";
1128              exit(1);                            //exit the program
1129          }
1130
1131          cout << "Please enter the name of the .pdb file: ";
1132
1133
1134          cin >> proton_distances_file;
1135          proton_distances.open(proton_distances_file);
1136          if(proton_distances.fail())             //if file does not open
```

```
1137            {                                       //inform the user
1138                cout << "The input file could not be opened.\n";
1139                exit(1);                            //exit the program
1140            }
1141
1142            cout << "Please enter a name for the output file: ";
1143
1144
1145            cin >> AssignedPeaksFile;
1146            AssignedPeaks.open(AssignedPeaksFile);
1147            if(AssignedPeaks.fail())                //if file does not open
1148            {                                       //inform the user
1149                cout << "The output file could not be opened.\n";
1150                exit(1);                            //exit the program
1151            }
1152        }
1153    else
1154        {
1155        int cshift_found = 0;
1156        int proton_found = 0;
1157        int assign_found = 0;
1158        int threed_found = 0;
1159
1160
1161        for(int i = 1; i < argc; i++)
1162            {
1163            if((argv[i][0] == '-') && (argv[i][1] == 'c'))
1164                {
1165                cshift_found = i+1;
1166                }
1167            if((argv[i][0] == '-') && (argv[i][1] == 'p'))
1168                {
1169                proton_found = i+1;
1170                }
1171            if((argv[i][0] == '-') && (argv[i][1] == 'o'))
1172                {
1173                assign_found = i+1;
1174                }
1175            if((argv[i][0] == '-') && (argv[i][1] == 't'))
1176                {
1177                threed_found = i+1;
1178                }
1179            }
1180
1181        if(threed_found == 0)
1182            {
1183            cout << "Please enter the name of the file containing";
1184            cout << " 3D NOE peak information: ";
1185            cin >> threeD_NOEInfoFile;
1186            threeD_NOEInfo.open(threeD_NOEInfoFile);
1187            }
1188        else
1189            {
1190            threeD_NOEInfo.open(argv[threed_found]);
1191            }
1192        if(threeD_NOEInfo.fail())                   //if file does not open
1193            {                                       //inform the user
1194                cout << "The input file could not be opened.\n";
1195                exit(1);                            //exit the program
1196            }
1197
1198        if(cshift_found == 0)
1199            {
1200            cout << "Please enter the name of the chemical shift file: ";
1201            cin >> ChemShiftFile;
1202            ChemShift.open(ChemShiftFile);
1203            }
1204        else
1205            {
1206            ChemShift.open(argv[cshift_found]);
1207            }
```

```
1208
1209      if(ChemShift.fail())                          //if file does not open
1210          {                                         //inform the user
1211              cout << "The input file could not be opened.\n";
1212              exit(1);                              //exit the program
1213          }
1214
1215      if(proton_found == 0)
1216          {
1217          cout << "Please enter the name of the .pdb file: ";
1218          cin >> proton_distances_file;
1219          proton_distances.open(proton_distances_file);
1220          }
1221      else
1222          {
1223          proton_distances.open(argv[proton_found]);
1224          }
1225
1226      if(proton_distances.fail())                   //if file does not open
1227          {                                         //inform the user
1228              cout << "The input file could not be opened.\n";
1229              exit(1);                              //exit the program
1230
1231          }
1232      if(assign_found == 0)
1233          {
1234          cout << "Please enter a name for the output file: ";
1235          cin >> AssignedPeaksFile;
1236          AssignedPeaks.open(AssignedPeaksFile);
1237          }
1238      else
1239          {
1240          AssignedPeaks.open(argv[assign_found]);
1241          }
1242
1243      if(AssignedPeaks.fail())                      //if file does not open
1244          {                                         //inform the user
1245              cout << "The output file could not be opened.\n";
1246              exit(1);                              //exit the program
1247          }                                         // end file check
1248
1249      }                                             // end else block
1250
1251
1252      int j = 0;
1253      char input;
1254
1255      if(verbose == 1)
1256      {
1257          cout << "Now reading Chemical Shift file into memory.\n";
1258      }
1259      while(input != '\n')
1260      {
1261          ChemShift.get(input);
1262      }
1263
1264      int meaningful_data = 0;
1265      while (!(ChemShift.eof()))
1266      {
1267          while(meaningful_data == 0)
1268          {
1269              input = ChemShift.peek();
1270              if(input == ' ' || input == '\t' || input == '\n')
1271                  ChemShift.get(input);
1272              else
1273                  meaningful_data = 1;
1274          }
1275          ChemShift >> ResidueName[j];
1276          meaningful_data = 0;
1277
1278          while(meaningful_data == 0)
```

```
1279          {
1280              input = ChemShift.peek();
1281              if(input == ' ' || input == '\t' || input == '\n')
1282                  ChemShift.get(input);
1283              else
1284                  meaningful_data = 1;
1285          }
1286          ChemShift >> ResidueNumber[j];
1287          meaningful_data = 0;
1288
1289          while(meaningful_data == 0)
1290          {
1291              input = ChemShift.peek();
1292              if(input == ' ' || input == '\t' || input == '\n')
1293                  ChemShift.get(input);
1294              else
1295                  meaningful_data = 1;
1296          }
1297          ChemShift >> AtomName[j];
1298          meaningful_data = 0;
1299
1300          while(meaningful_data == 0)
1301          {
1302              input = ChemShift.peek();
1303              if(input == ' ' || input == '\t' || input == '\n')
1304                  ChemShift.get(input);
1305              else
1306                  meaningful_data = 1;
1307          }
1308          ChemShift >> ppm[j];
1309          meaningful_data = 0;
1310
1311
1312          while(meaningful_data == 0)
1313          {
1314              input = ChemShift.peek();
1315              if(input == ' ' || input == '\t' || input == '\n')
1316                  ChemShift.get(input);
1317              else
1318                  meaningful_data = 1;
1319          }
1320          ChemShift >> order[j];
1321          meaningful_data = 0;
1322
1323          j++;
1324      }
1325
1326      j--;
1327
1328      int Array_Size_peaklist = j;
1329      if(verbose == 1)
1330      {
1331          cout << Array_Size_peaklist << " atoms read from";
1332          cout << " the Chemical Shift file.\n";
1333      }
1334
1335
1336      j = 0;
1337      input = 't';
1338
1339
1340      if(verbose == 1)
1341      {
1342          cout << "Now reading the 3D NOE Info file into memory.";
1343          cout << endl;
1344      }
1345      while(input != '\n')
1346      {
1347          threeD_NOEInfo.get(input);
1348      }
1349
```

```
1350      meaningful_data = 0;
1351      while (!(threeD_NOEInfo.eof()))
1352      {
1353          while(meaningful_data == 0)
1354          {
1355              input = threeD_NOEInfo.peek();
1356              if(input == ' ' || input == '\t' || input == '\n')
1357                  threeD_NOEInfo.get(input);
1358              else
1359                  meaningful_data = 1;
1360          }
1361          threeD_NOEInfo >> PeakNumber[j];
1362          meaningful_data = 0;
1363
1364          while(meaningful_data == 0)
1365          {
1366              input = threeD_NOEInfo.peek();
1367              if(input == ' ' || input == '\t' || input == '\n')
1368                  threeD_NOEInfo.get(input);
1369              else
1370                  meaningful_data = 1;
1371          }
1372          threeD_NOEInfo >> ppm1[j];
1373          meaningful_data = 0;
1374
1375          while(meaningful_data == 0)
1376          {
1377              input = threeD_NOEInfo.peek();
1378              if(input == ' ' || input == '\t' || input == '\n')
1379                  threeD_NOEInfo.get(input);
1380              else
1381                  meaningful_data = 1;
1382          }
1383          threeD_NOEInfo >> ppm2[j];
1384          meaningful_data = 0;
1385
1386          while(meaningful_data == 0)
1387          {
1388              input = threeD_NOEInfo.peek();
1389              if(input == ' ' || input == '\t' || input == '\n')
1390                  threeD_NOEInfo.get(input);
1391              else
1392                  meaningful_data = 1;
1393          }
1394          threeD_NOEInfo >> ppm3[j];
1395          meaningful_data = 0;
1396
1397
1398          while(meaningful_data == 0)
1399          {
1400              input = threeD_NOEInfo.peek();
1401              if(input == ' ' || input == '\t' || input == '\n')
1402                  threeD_NOEInfo.get(input);
1403              else
1404                  meaningful_data = 1;
1405          }
1406          threeD_NOEInfo >> PeakVolume[j];
1407          meaningful_data = 0;
1408
1409          j++;
1410      }
1411
1412      j--;
1413      int Array_Size_3Dfile  = j;
1414      if(verbose == 1)
1415      {
1416          cout << Array_Size_3Dfile << " 3D NOE peaks read";
1417          cout << " into memory from 3D NOE info file.\n";
1418      }
1419      j = 0;
1420      input = 't';
```

```
1421
1422
1423        if(verbose == 1)
1424        {
1425            cout << "Now reading Proton Distances file into memory.";
1426            cout << endl;
1427        }
1428        while(input != '\n')
1429        {
1430            proton_distances.get(input);
1431        }
1432
1433        meaningful_data = 0;
1434        while (!(proton_distances.eof()))
1435        {
1436            while(meaningful_data == 0)
1437            {
1438                input = proton_distances.peek();
1439                if(input == ' ' || input == '\t' || input == '\n')
1440                    proton_distances.get(input);
1441                else
1442                    meaningful_data = 1;
1443            }
1444            proton_distances >> pdbAtm[j];
1445            meaningful_data = 0;
1446
1447            while(meaningful_data == 0)
1448            {
1449                input = proton_distances.peek();
1450                if(input == ' ' || input == '\t' || input == '\n')
1451                    proton_distances.get(input);
1452                else
1453                    meaningful_data = 1;
1454            }
1455            proton_distances >> pdbAtmNum[j];
1456            meaningful_data = 0;
1457
1458            while(meaningful_data == 0)
1459            {
1460                input = proton_distances.peek();
1461                if(input == ' ' || input == '\t' || input == '\n')
1462                    proton_distances.get(input);
1463                else
1464                    meaningful_data = 1;
1465            }
1466            proton_distances >> pdbAtmNam[j];
1467            meaningful_data = 0;
1468
1469            while(meaningful_data == 0)
1470            {
1471                input = proton_distances.peek();
1472                if(input == ' ' || input == '\t' || input == '\n')
1473                    proton_distances.get(input);
1474                else
1475                    meaningful_data = 1;
1476            }
1477            proton_distances >> pdbResNam[j];
1478            meaningful_data = 0;
1479
1480
1481            while(meaningful_data == 0)
1482            {
1483                input = proton_distances.peek();
1484                if(input == ' ' || input == '\t' || input == '\n')
1485                    proton_distances.get(input);
1486                else
1487                    meaningful_data = 1;
1488            }
1489            proton_distances >> pdbResNum[j];
1490            meaningful_data = 0;
1491
```

```
1492            while(meaningful_data == 0)
1493            {
1494                input = proton_distances.peek();
1495                if(input == ' ' || input == '\t' || input == '\n')
1496                    proton_distances.get(input);
1497                else
1498                    meaningful_data = 1;
1499            }
1500            proton_distances >> pdbX[j];
1501            meaningful_data = 0;
1502
1503            while(meaningful_data == 0)
1504            {
1505                input = proton_distances.peek();
1506                if(input == ' ' || input == '\t' || input == '\n')
1507                    proton_distances.get(input);
1508                else
1509                    meaningful_data = 1;
1510            }
1511            proton_distances >> pdbY[j];
1512            meaningful_data = 0;
1513
1514
1515            while(meaningful_data == 0)
1516            {
1517                input = proton_distances.peek();
1518                if(input == ' ' || input == '\t' || input == '\n')
1519                    proton_distances.get(input);
1520                else
1521                    meaningful_data = 1;
1522            }
1523            proton_distances >> pdbZ[j];
1524            meaningful_data = 0;
1525
1526            while(meaningful_data == 0)
1527            {
1528                input = proton_distances.peek();
1529                if(input == ' ' || input == '\t' || input == '\n')
1530                    proton_distances.get(input);
1531                else
1532                    meaningful_data = 1;
1533            }
1534            proton_distances >> pdbFoo[j];
1535            meaningful_data = 0;
1536
1537            while(meaningful_data == 0)
1538            {
1539                input = proton_distances.peek();
1540                if(input == ' ' || input == '\t' || input == '\n')
1541                    proton_distances.get(input);
1542                else
1543                    meaningful_data = 1;
1544            }
1545            proton_distances >> pdbBar[j];
1546            meaningful_data = 0;
1547
1548            j++;
1549        }
1550
1551        j--;
1552
1553
1554        int Array_Size_pdbfile = j;
1555        if(verbose == 1)
1556        {
1557            cout << Array_Size_3Dfile << " atoms found in";
1558            cout << " proton distances file and read.\n";
1559        }
1560
1561        for (int i=0; i<= j; i++)
1562        {
```

```
1563            Exp_Assign[i] = -5;
1564        }
1565
1566    for(int i = 0; i < Array_Size_peaklist; i++)
1567        {
1568        if(AtomName[i] == "N")
1569            {
1570                AtomName[i] = "15N";
1571                ResidueNumber[i] = (ResidueNumber[i] / 100);
1572            }
1573        }
1574    for(int i = 0; i < Array_Size_pdbfile; i++)
1575        {
1576            if(pdbAtmNam[i] == "H")
1577            {
1578                pdbAtmNam[i] = "HN";
1579            }
1580            else if (pdbAtmNam[i] == "H1")
1581            {
1582                pdbAtmNam[i] = "HN";
1583            }
1584            else if (pdbAtmNam[i] == "1H")
1585            {
1586                pdbAtmNam[i] = "HT1";
1587            }
1588            else if (pdbAtmNam[i] == "1HA")
1589            {
1590                pdbAtmNam[i] = "HA";
1591            }
1592            else if (pdbAtmNam[i] == "1HB")
1593            {
1594                pdbAtmNam[i] = "HB";
1595            }
1596            else if (pdbAtmNam[i] == "1HG")
1597            {
1598                pdbAtmNam[i] = "HG";
1599            }
1600            else if (pdbAtmNam[i] == "1HD")
1601            {
1602                pdbAtmNam[i] = "HD";
1603            }
1604            else if (pdbAtmNam[i] == "1HD1")
1605            {
1606                pdbAtmNam[i] = "HD11";
1607            }
1608            else if (pdbAtmNam[i] == "1HD2")
1609            {
1610                pdbAtmNam[i] = "HD21";
1611            }
1612            else if (pdbAtmNam[i] == "1HE")
1613            {
1614                pdbAtmNam[i] = "HE";
1615            }
1616            else if (pdbAtmNam[i] == "1HE2")
1617            {
1618                pdbAtmNam[i] = "HE21";
1619            }
1620            else if (pdbAtmNam[i] == "1HZ")
1621            {
1622                pdbAtmNam[i] = "HZ";
1623            }
1624            else if (pdbAtmNam[i] == "1HG1")
1625            {
1626                pdbAtmNam[i] = "HG11";
1627            }
1628            else if (pdbAtmNam[i] == "1HG2")
1629            {
1630                pdbAtmNam[i] = "HG21";
1631            }
1632            else if (pdbAtmNam[i] == "1HH1")
1633            {
```

```
1634            pdbAtmNam[i] = "HH11";
1635        }
1636        else if (pdbAtmNam[i] == "1HH2")
1637        {
1638            pdbAtmNam[i] = "HH21";
1639        }
1640        else if (pdbAtmNam[i] == "2H")
1641        {
1642            pdbAtmNam[i] = "HT2";
1643        }
1644        else if (pdbAtmNam[i] == "1A")
1645        {
1646            pdbAtmNam[i] = "HA2";
1647        }
1648        else if (pdbAtmNam[i] == "2HB")
1649        {
1650            pdbAtmNam[i] = "HB2";
1651        }
1652        else if (pdbAtmNam[i] == "2HG")
1653        {
1654            pdbAtmNam[i] = "HG2";
1655        }
1656        else if (pdbAtmNam[i] == "2HD")
1657        {
1658            pdbAtmNam[i] = "HD2";
1659        }
1660        else if (pdbAtmNam[i] == "2HD1")
1661        {
1662            pdbAtmNam[i] = "HD12";
1663        }
1664        else if (pdbAtmNam[i] == "2HD2")
1665        {
1666            pdbAtmNam[i] = "HD22";
1667        }
1668        else if (pdbAtmNam[i] == "2HE")
1669        {
1670            pdbAtmNam[i] = "HE2";
1671        }
1672        else if (pdbAtmNam[i] == "2HE2")
1673        {
1674            pdbAtmNam[i] = "HE22";
1675        }
1676        else if (pdbAtmNam[i] == "2HZ")
1677        {
1678            pdbAtmNam[i] = "HZ2";
1679        }
1680        else if (pdbAtmNam[i] == "2HG1")
1681        {
1682            pdbAtmNam[i] = "HG12";
1683        }
1684        else if (pdbAtmNam[i] == "2HG2")
1685        {
1686            pdbAtmNam[i] = "HG22";
1687        }
1688        else if (pdbAtmNam[i] == "2HH1")
1689        {
1690            pdbAtmNam[i] = "HH12";
1691        }
1692        else if (pdbAtmNam[i] == "2HH2")
1693        {
1694            pdbAtmNam[i] = "HH22";
1695        }
1696        else if (pdbAtmNam[i] == "3HB")
1697        {
1698            pdbAtmNam[i] = "HB1";
1699        }
1700        else if (pdbAtmNam[i] == "3HG")
1701        {
1702            pdbAtmNam[i] = "HG1";
1703        }
1704        else if (pdbAtmNam[i] == "3HD")
```

```
1705            {
1706                pdbAtmNam[i] = "HD1";
1707            }
1708            else if (pdbAtmNam[i] == "3HE")
1709            {
1710                pdbAtmNam[i] = "HE1";
1711            }
1712            else if (pdbAtmNam[i] == "3HZ")
1713            {
1714                pdbAtmNam[i] = "HZ1";
1715            }
1716            else if (pdbAtmNam[i] == "3HG1")
1717            {
1718                pdbAtmNam[i] = "HG13";
1719            }
1720            else if (pdbAtmNam[i] == "?HG2")
1721            {
1722                pdbAtmNam[i] = "HG23";
1723            }
1724            else if (pdbAtmNam[i] == "3HD1")
1725            {
1726                pdbAtmNam[i] = "HD13";
1727            }
1728            else if (pdbAtmNam[i] == "3HD2")
1729            {
1730                pdbAtmNam[i] = "HD23";
1731            }
1732        }
1733
1734
1735    int count = 0;
1736        if(verbose == 1)
1737        {
1738            cout << "Now making D1 assignments by comparing the";
1739            cout << " PPM1 value specified in the 3D NOE Info file";
1740            cout << " to the PPM value specified in the Chemical";
1741            cout << " Shift file. If their absolute value is less";
1742            cout << " than the D1 uncertainty, a match is";
1743            cout << " identified.\n";
1744        }
1745    for(int i = 0; i < Array_Size_3Dfile; i++)
1746        {
1747        count = 0;
1748        for(int j = 0; j <= Array_Size_peaklist; j++)
1749            {
1750            if((fabs(ppm1[i] - ppm[j])) <= D1_UNCERTAINTY)
1751                {
1752                d1_assigns[i][count] = j;
1753                d1_reverse_assigns[j][count] = i;
1754                count++;
1755                total_assigns_made++;
1756                }
1757
1758            }
1759        counts_d1[i] = count;
1760        }
1761    D1_matches = total_assigns_made;
1762
1763        if(verbose == 1)
1764        {
1765            cout << D1_matches << " assignments made based on";
1766            cout << " the ppm1 values.\n";
1767        }
1768
1769    total_assigns_made = 0;
1770
1771        if(verbose == 1)
1772        {
1773            cout << "Now making D3 assignments by comparing the PPM3";
1774            cout << " value specified in the 3D NOE Info file to the";
1775            cout << " PPM value specified in the Chemical Shift file.";
```

```
1776            cout << " If their absolute value is less than the D3";
1777            cout << " uncertainty, a match is identified.\n";
1778        }
1779    for(int i = 0; i < Array_Size_3Dfile; i++)
1780        {
1781
1782        count = 0;
1783        for(int j = 0; j <= Array_Size_peaklist; j++)
1784            {
1785            if((fabs(ppm3[i] - ppm[j])) <= D3_UNCERTAINTY)
1786                {
1787                d3_assigns[i][count] = j;
1788                d3_reverse_assigns[j][count] = i;
1789                count++;
1790                total_assigns_made++;
1791                }
1792            }
1793        counts_d3[i] = count;
1794        }
1795
1796    D3_matches = total_assigns_made;
1797
1798        if(verbose == 1)
1799        {
1800            cout << D3_matches << " assignments made based on";
1801            cout << " the ppm3 values.\n";
1802        }
1803
1804
1805
1806
1807        if(verbose == 1)
1808        {
1809            cout << "Now making D2 assignments by comparing the PPM2";
1810            cout << " value specified in the 3D NOE Info file to the";
1811            cout << " PPM value specified in the Chemical Shift file.";
1812            cout << " If their absolute value is less than the D2";
1813            cout << " uncertainty, a match is identified.\n";
1814        }
1815
1816    total_assigns_made = 0;
1817
1818    for(int i = 0; i < Array_Size_3Dfile; i++)
1819        {
1820        count = 0;
1821        for(int j = 0; j <= Array_Size_peaklist; j++)
1822            {
1823            if((fabs(ppm2[i] - ppm[j])) <= D2_UNCERTAINTY)
1824                {
1825                d2_assigns[i][count] = j;
1826                d2_reverse_assigns[j][count] = i;
1827                count++;
1828                total_assigns_made++;
1829                }
1830            }
1831            counts_d2[i] = count;
1832
1833        }
1834
1835        if(verbose == 1)
1836        {
1837            cout << total_assigns_made << " assignments made based";
1838            cout << " on the ppm3 values.\n";
1839        }
1840
1841
1842
1843    // calculate distances
1844
1845    double pdb_X1 = 0.00;
1846    double pdb_Y1 = 0.00;
```

```
1847  double pdb_Z1 = 0.00;
1848  double pdb_X2 = 0.00;
1849  double pdb_Y2 = 0.00;
1850  double pdb_Z2 = 0.00;
1851                  //initialize variables in distance formula to 0
1852
1853
1854
1855  if(verbose == 1)
1856      {
1857          cout << "Now making distance calculations for all atoms";
1858          cout << " in the PDB file.\n";
1859      }
1860
1861  int print_distances = 0;
1862  if(argc > 1)
1863      {
1864          for(int y = 0; y < argc; y++)
1865          {
1866              if(argv[y][0] == '-' && argv[y][1] == 'd')
1867              {
1868                  print_distances = 1;
1869              }
1870          }
1871      }
1872
1873  if(print_distances == 0)
1874      {
1875      for(int u = 0; u < Array_Size_pdbfile; u++)
1876          {
1877          pdb_X1 = pdbX[u];
1878          pdb_Y1 = pdbY[u];
1879          pdb_Z1 = pdbZ[u];
1880
1881          for(int v = 0; v < Array_Size_pdbfile; v++)
1882              {
1883              if(u != v)                  //if the protons are two
1884                  {                       //different protons, use
1885                  pdb_X2 = pdbX[v];       //distance formula to
1886                  pdb_Y2 = pdbY[v];       //calculate distance
1887                  pdb_Z2 = pdbZ[v];       //between them
1888                  distances[u][v] = sqrt(pow((pdb_X1 - pdb_X2),2) +
1889                                         pow((pdb_Y1-pdb_Y2),2) +
1890                                        pow((pdb_Z1 - pdb_Z2),2));
1891                  }
1892              else
1893                  distances[u][v] = 0.00;
1894              } //else distance is between the proton and itself
1895          }
1896                  //repeat calculations; calculate distance
1897                  //between each proton and every other proton
1898      }
1899
1900  else
1901      {
1902      AssignedPeaks << "Distances:\n";
1903      for(int u = 0; u < Array_Size_pdbfile; u++)
1904          {
1905          pdb_X1 = pdbX[u];
1906          pdb_Y1 = pdbY[u];
1907          pdb_Z1 = pdbZ[u];
1908
1909          for(int v = 0; v < Array_Size_pdbfile; v++)
1910              {
1911              if(u != v)                  //if the protons are two
1912              {                           //different protons, use the
1913              pdb_X2 = pdbX[v];           //distance formula to calculate
1914              pdb_Y2 = pdbY[v];           //calculate the distance
1915              pdb_Z2 = pdbZ[v];           //between them
1916              AssignedPeaks << setiosflags(ios::showpoint);
1917              AssignedPeaks << setiosflags( ios::fixed );
```

```
1918                AssignedPeaks << setprecision(3);
1919                AssignedPeaks << pdbAtmNum[u] << "\t" << pdbAtmNam[u];
1920                AssignedPeaks << "\t" << pdbResNam[u] << "\t";
1921                AssignedPeaks << pdbResNum[u] << "\tX=" << pdbX[u];
1922                AssignedPeaks << "\tY=" << pdbY[u] << "\tZ=";
1923                AssignedPeaks << pdbZ[u] << "\n" << pdbAtmNum[v];
1924                AssignedPeaks << "\t" << pdbAtmNam[v] << "\t";
1925                AssignedPeaks << pdbResNum[v] << "\t" << pdbResNum[v];
1926                AssignedPeaks << "\tX=" << pdbX[v] << "\tY=";
1927                AssignedPeaks << pdbY[v] << "\tZ=" << pdbZ[v] << "\n";
1928                distances[u][v] = sqrt(pow((pdb_X1 - pdb_X2),2) +
1929                                       pow((pdb_Y1-pdb_Y2),2) +
1930                                    pow((pdb_Z1 - pdb_Z2),2));
1931                AssignedPeaks << "Distance: " << distances[u][v];
1932                AssignedPeaks << endl;
1933
1934                }
1935                else
1936                    distances[u][v] = 0.00;
1937                }   //else distance is between the proton and itself
1938            }
1939                //repeat calculations; calculate distance
1940                //between each proton and every other proton
1941        }
1942
1943
1944
1945
1946    D2_matches = count;
1947    cout.setf(ios::fixed);
1948    cout.setf(ios::showpoint);          //format numbers for output
1949
1950
1951
1952    int temp_y = 0;
1953
1954        if(verbose == 1)
1955        {
1956            cout << "Printing assignments to the output file.\n";
1957        }
1958    for(int i = 0; i < Array_Size_3Dfile; i++)
1959        {
1960
1961        if((d1_assigns[i][0] != -5) && (d3_assigns[i][0] != -5) &&
1962            (d2_assigns[i][0] != -5 && d2_assigns[i][1] == -5))
1963            {
1964            if(temp_y == 0)
1965            {
1966                AssignedPeaks << "Unambigously Assigned: " << endl;
1967                AssignedPeaks << "PeakNum" << "\t" << "Name" << "\t";
1968                AssignedPeaks << "ResNum" << "\t" << "AtmName";
1969                AssignedPeaks << "\t" << "Shift" << "\t";
1970                AssignedPeaks << "D1Shift" << "\t" << "Name" << "\t";
1971                AssignedPeaks << "ResNum" << "\t" << "AtmName";
1972                AssignedPeaks << "\t" << "Shift" << "\t";
1973                AssignedPeaks << "D2Shift" << "\t" << "Name" << "\t";
1974                AssignedPeaks << "ResNum" << "\t" << "AtmName";
1975                AssignedPeaks << "\t" << "Shift" << "\t";
1976                AssignedPeaks << "D3Shift" << "\t" << "Distance" << endl;
1977                temp_y++;
1978            }
1979            int column = 0;
1980            int column2 = 0;
1981            while(d1_assigns[i][column] != -5)
1982            {
1983                while(d3_assigns[i][column2] != -5)
1984                {
1985                    if(ResidueNumber[d1_assigns[i][column]] ==
1986                       ResidueNumber[d3_assigns[i][column2]] &&
1987                       d1_assigns[i][column] >= 0 &&
1988                       d2_assigns[i][0] >= 0 &&
```

```
                    d3_assigns[i][column2] >= 0)
                {

                for (int j = 0; j < Array_Size_pdbfile; j++)
                {
                if (ResidueNumber[d1_assigns[i][column]] ==
                    pdbResNum[j] &&
                    AtomName[d1_assigns[i][column]] ==
                    pdbAtmNam[j])
                {
                    X1 = pdbX[j];
                    Y1 = pdbY[j];
                    Z1 = pdbZ[j];
                }
                if (ResidueNumber[d2_assigns[i][0]] ==
                    pdbResNum[j] &&
                    AtomName[d2_assigns[i][0]] ==
                    pdbAtmNam[j])
                {
                    X2 = pdbX[j];
                    Y2 = pdbY[j];
                    Z2 = pdbZ[j];
                }

            }
            Atom_Distance = sqrt(pow((X1 - X2),2) +
                                 pow((Y1 - Y2),2) +
                                 pow((Z1 - Z2),2));

            AssignedPeaks << PeakNumber[i] << "\t";
            AssignedPeaks << ResidueName[d1_assigns[i][column]] << "\t";
            AssignedPeaks << ResidueNumber[d1_assigns[i][column]] << "\t";
            AssignedPeaks << AtomName[d1_assigns[i][column]] << "\t";
            AssignedPeaks << setprecision(6) << ppm[d1_assigns[i][column]];
            AssignedPeaks << "\t" << ppm1[i];
            AssignedPeaks << "\t" << ResidueName[d2_assigns[i][0]];
            AssignedPeaks << "\t" << ResidueNumber[d2_assigns[i][0]];
            AssignedPeaks << "\t" << AtomName[d2_assigns[i][0]];
            AssignedPeaks << "\t" << ppm[d2_assigns[i][0]];
            AssignedPeaks << "\t" << ppm2[i] << "\t";
            AssignedPeaks << ResidueName[d3_assigns[i][column2]] << "\t";
            AssignedPeaks << ResidueNumber[d3_assigns[i][column2]] << "\t";
            AssignedPeaks << AtomName[d3_assigns[i][column2]] << "\t";
            AssignedPeaks << ppm[d3_assigns[i][column2]] << "\t";
            AssignedPeaks << ppm3[i] << "\t" << Atom_Distance << endl;

                } //end if statement
            column2++;
            } //end inner while loop
        column++;
        } //end outer while loop
        }
    }
    AssignedPeaks <<  endl;
                        //if there is one assignment in D1, D2
                        //and D3 dimensions AND if D1 assignment
                        //matches D1 assignment, print residue
                        //with chemical shift assignments


cout.setf(ios::fixed);
cout.setf(ios::showpoint);        //format numbers for output

AssignedPeaks << "Unassigned, No D1 assignment: " << endl;
AssignedPeaks << "PeakNum" << "\t";
AssignedPeaks << "D1Shift" << "\t" << "Name";
AssignedPeaks << "\t" << "ResNum" << "\t" << "AtmName" << "\t";
AssignedPeaks << "Shift" << "\t" << "D2Shift" << "\t";
AssignedPeaks << "Name" << "\t" << "ResNum";
AssignedPeaks << "\t" << "AtmName" << "\t" << "Shift";
```

```
2060  AssignedPeaks << "\t" << "D3Shift" << endl;
2061
2062  for(int i = 0; i < Array_Size_3Dfile; i++)
2063      {
2064      if (d2_assigns[i][0] >= 0 && d3_assigns[i][0] >= 0)
2065      {
2066          if(d1_assigns[i][0] == -5)
2067          {
2068          AssignedPeaks << PeakNumber[i] << "\t" << ppm1[i];
2069          AssignedPeaks << "\t" << ResidueName[d2_assigns[i][0]];
2070          AssignedPeaks << "\t" << ResidueNumber[d2_assigns[i][0]];
2071          AssignedPeaks << "\t" << AtomName[d2_assigns[i][0]];
2072          AssignedPeaks << setprecision(6);
2073          AssignedPeaks << "\t" << ppm[d2_assigns[i][0]];
2074          AssignedPeaks << "\t" << ppm2[i] << "\t";
2075          AssignedPeaks << ResidueName[d3_assigns[i][0]] << "\t";
2076          AssignedPeaks << ResidueNumber[d3_assigns[i][0]] << "\t";
2077          AssignedPeaks << AtomName[d3_assigns[i][0]] << "\t";
2078          AssignedPeaks << ppm[d3_assigns[i][0]] << "\t";
2079          AssignedPeaks << ppm3[i] << endl;
2080
2081          }
2082      }
2083      }
2084      AssignedPeaks <<  endl;
2085                      //if first value in D1 assigned array
2086                      //has not been reassigned, no other
2087                      //values in array have been reassigned
2088                      //the residue has no D1 assignment, print
2089                      //residue with chemical shift assignments
2090
2091  AssignedPeaks <<  "Unassigned, No D2 assignment: " << endl;
2092  AssignedPeaks << "PeakNum" << "\t" << "D2Shift" << "\t" << "Name";
2093  AssignedPeaks << "\t" << "ResNum" << "\t" << "AtmName" << "\t";
2094  AssignedPeaks << "Shift" << "\t" << "D1Shift" << "\t";
2095  AssignedPeaks << "Name" << "\t" << "ResNum" << "\t" << "AtmName";
2096  AssignedPeaks << "\t" << "Shift" << "\t" << "D3Shift" << endl;
2097
2098  for(int i = 0; i < Array_Size_3Dfile; i++)
2099      {
2100      if (d1_assigns[i][0] >= 0 && d3_assigns[i][0] >= 0)
2101      {
2102          if(d2_assigns[i][0] == -5)
2103          {
2104          AssignedPeaks << PeakNumber[i] << "\t" << ppm2[i];
2105          AssignedPeaks << "\t" << ResidueName[d1_assigns[i][0]];
2106          AssignedPeaks << "\t" << ResidueNumber[d1_assigns[i][0]];
2107          AssignedPeaks << "\t" << AtomName[d1_assigns[i][0]];
2108          AssignedPeaks << setprecision(6);
2109          AssignedPeaks << "\t" << ppm[d1_assigns[i][0]];
2110          AssignedPeaks << "\t" << ppm1[i] << "\t";
2111          AssignedPeaks << ResidueName[d3_assigns[i][0]] << "\t";
2112          AssignedPeaks << ResidueNumber[d3_assigns[i][0]] << "\t";
2113          AssignedPeaks << AtomName[d3_assigns[i][0]] << "\t";
2114          AssignedPeaks << ppm[d3_assigns[i][0]] << "\t";
2115          AssignedPeaks << ppm3[i] << endl;
2116          }
2117      }
2118      }
2119  AssignedPeaks <<  endl;
2120                  //if first value in D2 assigned array
2121                  //has not been reassigned, no other
2122                  //values in array have been reassigned;
2123                  //the residue has no D2 assignment, print
2124                  //residue with chemical shift assignments
2125
2126
2127  AssignedPeaks << "Unassigned, No D3 assignment: " << endl;
2128  AssignedPeaks << "PeakNum" << "\t" << "D3Shift" << "\t" << "Name";
2129  AssignedPeaks << "\t" << "ResNum" << "\t" << "AtmName" << "\t";
2130  AssignedPeaks << "Shift" << "\t" << "D1Shift" << "\t";
```

```
2131 AssignedPeaks << "Name" << "\t" << "ResNum" << "\t";
2132 AssignedPeaks << "AtmName" << "\t" << "Shift" << "\t";
2133 AssignedPeaks << "D2Shift" << endl;
2134
2135 for(int i = 0; i < Array_Size_3Dfile; i++)
2136     {
2137     if (d1_assigns[i][0] >= 0 && d2_assigns[i][0] >= 0)
2138     {
2139         if(d3_assigns[i][0] == -5)
2140         {
2141         AssignedPeaks << PeakNumber[i] << "\t" << ppm3[i];
2142         AssignedPeaks << "\t" << ResidueName[d1_assigns[i][0]];
2143         AssignedPeaks << "\t" << ResidueNumber[d1_assigns[i][0]];
2144         AssignedPeaks << "\t" << AtomName[d1_assigns[i][0]];
2145         AssignedPeaks << setprecision(6);
2146         AssignedPeaks << "\t" << ppm[d1_assigns[i][0]];
2147         AssignedPeaks << "\t" << ppm1[i] << "\t";
2148         AssignedPeaks << ResidueName[d2_assigns[i][0]] << "\t";
2149         AssignedPeaks << ResidueNumber[d2_assigns[i][0]] << "\t";
2150         AssignedPeaks << AtomName[d2_assigns[i][0]] << "\t";
2151         AssignedPeaks << ppm[d2_assigns[i][0]] << "\t";
2152         AssignedPeaks << ppm2[i] << endl;
2153         }
2154     }
2155     }
2156 AssignedPeaks <<  endl;
2157                   //if first value in D3 assigned array
2158                   //has not been reassigned, no other
2159                   //values in array have been reassigned;
2160                   //the residue has no D3 assignment, print
2161                   //residue with chemical shift assignments
2162
2163
2164
2165 AssignedPeaks << "Unassigned, mismatch between D1";
2166 AssignedPeaks << " and D3 assignment: " << endl;
2167 AssignedPeaks << "PeakNum" << "\t" << "Name" << "\t";
2168 AssignedPeaks << "ResNum" << "\t" << "AtmName" << "\t";
2169 AssignedPeaks << "Shift" << "\t" << "D1Shift" << "\t";
2170 AssignedPeaks << "Name" << "\t" << "ResNum" << "\t";
2171 AssignedPeaks << "AtmName" << "\t" << "Shift" << "\t";
2172 AssignedPeaks << "D2Shift" << "\t";
2173 AssignedPeaks << "Name" << "\t" << "ResNum" << "\t";
2174 AssignedPeaks << "AtmName" << "\t" << "Shift" << "\t";
2175 AssignedPeaks << "D3Shift" << endl;
2176
2177 for(int i = 0; i < Array_Size_3Dfile; i++)
2178     {
2179
2180     if(ResidueNumber[d1_assigns[i][0]] !=
2181        ResidueNumber[d3_assigns[i][0]])
2182         {
2183         if (d1_assigns[i][0] >= 0 && d2_assigns[i][0] >= 0 &&
2184             d3_assigns[i][0] >= 0)
2185         {
2186         AssignedPeaks << PeakNumber[i] << "\t";
2187         AssignedPeaks << ResidueName[d1_assigns[i][0]] << "\t";
2188         AssignedPeaks << ResidueNumber[d1_assigns[i][0]] << "\t";
2189         AssignedPeaks << AtomName[d1_assigns[i][0]] << "\t";
2190         AssignedPeaks << setprecision(6) << ppm[d1_assigns[i][0]];
2191         AssignedPeaks << "\t" << ppm1[i];
2192         AssignedPeaks << "\t" << ResidueName[d2_assigns[i][0]];
2193         AssignedPeaks << "\t" << ResidueNumber[d2_assigns[i][0]];
2194         AssignedPeaks << "\t" << AtomName[d2_assigns[i][0]];
2195         AssignedPeaks << "\t" << ppm[d2_assigns[i][0]];
2196         AssignedPeaks << "\t" << ppm2[i] << "\t";
2197         AssignedPeaks << ResidueName[d3_assigns[i][0]] << "\t";
2198         AssignedPeaks << ResidueNumber[d3_assigns[i][0]] << "\t";
2199         AssignedPeaks << AtomName[d3_assigns[i][0]] << "\t";
2200         AssignedPeaks << ppm[d3_assigns[i][0]] << "\t";
2201         AssignedPeaks << ppm3[i] << endl;
```

```
2202          }
2203
2204          }
2205      }
2206      AssignedPeaks <<  endl;
2207                        //if D1 and D3 assignments do not
2208                        //match, print residue with chemical
2209                        //shift assignments
2210
2211  int d1_assignment_count = 0;
2212  int d2_assignment_count = 0;
2213  int d3_assignment_count = 0;
2214
2215  int not_found = 0;
2216  int temp_count = 0;
2217
2218  AssignedPeaks << "Ambiguous Assignment, multiple D2 assignments: ";
2219  AssignedPeaks << endl << "PeakNum" << "\t" << "Name" << "\t";
2220  AssignedPeaks << "ResNum" << "\t" << "AtmName" << "\t";
2221  AssignedPeaks << "Shift" << "\t" << "D1Shift" << "\t";
2222  AssignedPeaks << "Name" << "\t" << "ResNum" << "\t" << "AtmName";
2223  AssignedPeaks << "\t" << "Shift" << "\t" << "D2Shift" << "\t";
2224  AssignedPeaks << "Name" << "\t" << "ResNum" << "\t";
2225  AssignedPeaks << "AtmName" << "\t" << "Shift" << "\t";
2226  AssignedPeaks << "D3Shift" << "\t" << "Distance" << endl;
2227
2228  for(int i = 0; i < Array_Size_3Dfile; i++)
2229      {
2230      if((d2_assigns[i][0] != -5) && (d2_assigns[i][1] != -5))
2231      {
2232      int column = 0;
2233
2234          while(d2_assigns[i][column] != -5)
2235          {
2236              if(ResidueNumber[d1_assigns[i][0]] ==
2237                 ResidueNumber[d3_assigns[i][0]] &&
2238                 d1_assigns[i][0] >= 0 &&
2239                 d2_assigns[i][column] >= 0 && d3_assigns[i][0] >= 0)
2240              {
2241
2242              for (int j = 0; j < Array_Size_pdbfile; j++)
2243              {
2244                  if (ResidueNumber[d1_assigns[i][0]] ==
2245                      pdbResNum[j] &&
2246                      AtomName[d1_assigns[i][0]] ==
2247                      pdbAtmNam[j])
2248                  {
2249                      X1 = pdbX[j];
2250                      Y1 = pdbY[j];
2251                      Z1 = pdbZ[j];
2252                  }
2253                  if (ResidueNumber[d2_assigns[i][column]] ==
2254                      pdbResNum[j] &&
2255                      AtomName[d2_assigns[i][column]] ==
2256                      pdbAtmNam[j])
2257                  {
2258                      X2 = pdbX[j];
2259                      Y2 = pdbY[j];
2260                      Z2 = pdbZ[j];
2261                  }
2262
2263              }
2264              Atom_Distance = sqrt(pow((X1 - X2),2) +
2265                                   pow((Y1 - Y2),2) +
2266                                   pow((Z1 - Z2),2));
2267
2268
2269              AssignedPeaks << PeakNumber[i] << "\t";
2270              AssignedPeaks << ResidueName[d1_assigns[i][0]] << "\t";
2271              AssignedPeaks << ResidueNumber[d1_assigns[i][0]] << "\t";
2272              AssignedPeaks << AtomName[d1_assigns[i][0]] << "\t";
```

```
2273            AssignedPeaks << setprecision(6) << ppm[d1_assigns[i][0]];
2274            AssignedPeaks << "\t" << ppm1[i];
2275            AssignedPeaks << "\t" << ResidueName[d2_assigns[i][column]];
2276            AssignedPeaks << "\t" << ResidueNumber[d2_assigns[i][column]];
2277            AssignedPeaks << "\t" << AtomName[d2_assigns[i][column]];
2278            AssignedPeaks << "\t" << ppm[d2_assigns[i][column]];
2279            AssignedPeaks << "\t" << ppm2[i] << "\t";
2280            AssignedPeaks << ResidueName[d3_assigns[i][0]] << "\t";
2281            AssignedPeaks << ResidueNumber[d3_assigns[i][0]] << "\t";
2282            AssignedPeaks << AtomName[d3_assigns[i][0]] << "\t";
2283            AssignedPeaks << ppm[d3_assigns[i][0]] << "\t";
2284            AssignedPeaks << ppm3[i] << "\t" << setprecision(5);
2285            AssignedPeaks << Atom_Distance << endl;
2286            } //end inner if statement
2287
2288            column++;
2289
2290        } //end inner while loop
2291    } //end outer if statement
2292    }
2293
2294    if(verbose == 1)
2295    {
2296        cout << "Closing output file.\n";
2297    }
2298
2299    proton_distances.close();
2300    threeD_NOEInfo.close();
2301    ChemShift.close();                    //close input files
2302    AssignedPeaks.close();                //close output file
2303
2304 end_time = time(NULL);
2305
2306
2307 if(verbose == 1)
2308    {
2309        cout << "Program completed in ";
2310        cout << end_time - start_time;
2311        cout << " seconds.\n";
2312    }
2313 if(verbose == 1)
2314    {
2315        cout << "Program terminated normally.\n";
2316    }
2317 return 0;
2318 }  //end main
2319
2320
2321
2322
2323
2324
2325 void print_help()
2326 {
2327
2328    cout << "\nNOE(1)\n\n";
2329    cout << "NAME\n";
2330    cout << "\tnoe - make residue assignments using 3D";
2331    cout << " noe peaks and residue chemical shifts.";
2332    cout << "\n\nSYNOPSIS\n";
2333    cout << "noe \t[-c Chemical Shift file to use]";
2334    cout << " [-p pdbfile to use]\n";
2335    cout << "\t[-t 3D NOE info file to use]";
2336    cout << " [-o output file to write to]\n";
2337    cout << "\n\n\n";
2338    cout << "DESCRIPTION\n";
2339    cout << "\tWhen NOE is invoked, the files are";
2340    cout << " read in and based upon the standard\n";
2341    cout << "definitions, assignments of the residues";
2342    cout << " are made and outputted to the file.";
2343    cout << "\n";
```

```
2344      cout << "This program was created by Maura Mahar as";
2345      cout << " part of her senior research.\n\n";
2346
2347
2348  }
2349
```

Results

A sample output file is listed in the Appendix, section III. The output consists of a table of residue assignments for BYRubredoxin. The program was designed to assign each NOE peak and to sort each assignment into one of three categories: unambiguously assigned, ambiguously assigned, and unassigned peaks. Peaks are considered unambiguously assigned if there is only one assignment in the second dimension and if the assignment in the first dimension matches the assignment in the third dimension. Peaks are ambiguously assigned if the assignments in the first and third dimensions are the same but there is more than one possible assignment for the second dimension. Peaks are considered unassigned if there is no assignment in the first dimension and/or second dimension and/or third dimension, or if the assignments in the first and third dimensions do not match. Atom distances were calculated only for those peaks that were unambiguously or ambiguously assigned.

Discussion

The correctness of the program can be assessed by comparing the program's peak assignments to the assignments obtained by hand. Since a list of hand-assigned peaks was not available for BYRubredoxin, a list of hand-assigned peaks for A2K was used for comparison. In general, the program-assigned peaks matched the hand-assigned peaks.

All unambiguous, program-assigned peaks with atom distances calculated to be greater than 6.0Å were compared to the corresponding hand-assigned peaks. These assignments were singled out because protons that are more than 6.0Å from each other will not "see" each other and, therefore, should not produce an NOE peaks. Since these peaks fall into the unambiguously assigned category, they were compared to the hand-assigned peaks to determine why valid assignments are being made for atoms that are more than 6.0Å apart. Upon comparison to the hand-assigned peaks, the program-assigned peaks were divided into three categories: correctly assigned peaks, misassigned peaks, and very small peaks.

In the correctly assigned category, the program-assigned peaks matched the hand-assigned peaks, however, the atom distances differed, sometimes significantly, between the two sets. For all the peaks in this category, the atom distances calculated by the program were greater than 6.0Å, while the distances calculated from the NOE volumes were all less than 6.0Å. Each method of calculating atom distances is a valid, accurate method, indicating that discrepancies in the distances were due to an inaccuracy in the computer model of the protein. Since each atom in the protein has a set of x, y, and z coordinates, determining that an atom is incorrectly placed does not indicate what the correct placement might be. These discrepancies are, however, a place to start altering the model and correct for the inaccuracies.

The misassigned peaks category is for those program-assigned peaks that were assigned to the wrong atom in the second dimension. In each case, there were multiple valid assignments in the second dimension. The program was designed to choose the atom closest to the amide proton (according to the calculated distances) and assign it in the second dimension. According to the hand-assigned peaks, the correct assignment was to an atom further away. There are not many assigned peaks that fall into this category and there is not a fault of the program. In each case, the correct assignment had to be deduced using experimental spectra; a list of chemical shifts was not sufficient. Since the program makes assignments based solely on chemical shift comparisons, this category of assignments will always have to be compared by hand.

Peaks in the small peaks category are those program-assigned peaks with peak volumes that have been determined to be too small to be valid peaks. These peaks will also have to be examined by hand to determine whether these peaks are valid peaks or noise picked up during the experiment.

References

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Appendix

I. Protocol

The following is a protocol for determining low energy structures of BYRubredoxin which are close to the X-ray structures, 1BQ8.pdb (Pf, thermophile) and 5RXN.pdb (Cp, mesophile). Energy minimizations for other hybrid structures that are close to the X-ray structures of Pf and Cp can also be performed using the following protocol.

1. Remove chain identifier and water molecules from 1BQ8.pdb file.
   Remove protons and water molecules from 5RXN.pdb file.

2. Use Midas to overlap the two X-ray structures. To match all 54 residues using only the backbone atoms N, CA, C, and O:

   midas

   open 0 1BQ8.pdb
   open 1 5RXN.pdb
   match #0:1-54 mainchain #1:1-54 mainchain

   Write down the RMS error. The number of matched atoms should be the same.

   To match parts of the structure, for example, residues 11-13 and 38-40 using the backbone and sidechain atoms:

   match #0:11-13,38-40 #1:11-13,38-40

   Check to be sure the number of matched atoms is the same.

   Write out the matched coordinates (new file names will be 1BQ8_match.pdb and 5RXN_match.pdb):

   write 0 1BQ8_match.pdb
   write 1 5RXN_match.pdb

3. Create the hybrid protein by selecting residues from each matched .pdb file, and creating a new .pdb file. Be sure the Fe metal center is replaced with Zn and make sure the Zn atom is connected to the S atoms of Cys 6, 9, 39, and 42 (using the CONECT function at the end of the .pdb file).

4. Use the program **fixnumbers** to renumber the atoms in the merged .pdb file. Renumber the atoms, making sure the first atom has the number 1. Call this file "hybrid.pdb".

5. Use **maestro** (Macromodel) to calculate the overlap energy of the hybrid protein.

   Import hybrid.pdb into maestro as pdb file.

Fix the Zn atom by going to Edit/Build/Atoms/Atom Types and selecting Zn (87). Click on Retype, then left-mouse click on the Zn atom in the structure. The color should change from orange to blue.

Add hydrogens by going to Edit/Hydrogen Treatment. Select All-atom with S-Lp, which is appropriate for the Amber force field.

Fix the bond order between Zn and S by going to Edit/Bond Properties. Select zero order bond, and click on each Zn-S bond. The color should change from blue to green. It is helpful to enlarge the structure so that you can click on each bond precisely.

Check the geometry around the Zn.

The values should be:

bond angles:	CB-S1.Zn	105.2°
	S1.Zn.S1	109.5°
bond length:	Zn.S1	2.2900 Å

Use Edit/Adjust to fix distances and bond angles. For safety, use Edit/Begin Undo Block so that you can start over again if you have to.

* Select the **Distance** tab. Make sure the Allow Adjusting option is NOT highlighted (this will prevent you from accidentally clicking on the project screen and drastically changing a bond length/angle). Make sure Atoms is highlighted on the project screen under "Pick States." Click on 2 atoms, then go to the text box in the Adjust window next to "Distance" and type in the correct bond length according to the values listed from the crystallographic structure. Hit enter and note that the atoms involved in the change are listed in the text box above. Repeat this process for all bonds to be changed.

Now change the angles by selecting the **Angle** tab. Change the bond angles in the same manner as the bond lengths were changed. Use the angles listed from the crystallographic structure.

* Select the **Contacts** tab. Make sure the Show Markers option is highlighted and, since we are only interested in the bad contacts, make sure the Good Contacts option is NOT highlighted. Good contacts are shown in green, bad contacts as orange, and ugly contacts as red.

The value of each contact is determined as follows:

$$C = \frac{\text{Distance between atomic centers}}{\text{Radius first atom} + \text{Radius second atom}}$$

The value of C for each contact must increase from ugly to good. In other words,

$$C_{ugly} < C_{bad} < C_{good}$$

To find contacts, an atom set MUST be defined in Atom Set 1, but nothing has to be defined for Atom Set 2. To define an atom set, highlight the Pick To Add option under Atom Set 1 and click on an atom in the project screen. Note that contact lines appear

without having defined a second atom set. To define a second atom set, highlight the Pick To Add option under Atom Set 2 and click on an atom in the project screen.

If a second atom set is not defined, the contact lines shown are intra-contacts for all atoms in set 1. If a second atom set is defined, the contact lines shown are contacts from set 1 to set 2.

Calculate the current energy of the hybrid protein. Macromodel/Current Energy. Export resulting structure as an .m2 file.

Change charges in the .m2 file as follows:

Atom	Old Charge	New Charge		
Zn	2.00000	0.83160	x (1/4) =	0.20790
S	0.77698	-0.03022		-0.03022
LP	-0.38099	-0.38099	x (2) =	-0.76198
CB	0.04402	0.53570		0.53570
HB	0.04949	-0.14670	x (2) =	-0.29340

1/4 Zn + Cys sidechain =	-0.34200
+ Cys backbone =	-0.15800
Total for each Cys + (1/4) Zn =	-0.50000
	x 4
	-2.00000

Read the .m2 file (with new corrected charges) back into Macromodel.

6. When the charges have been corrected, read the .m2 file back into Macromodel and create the protein as a project. Project/Create Entry from Workspace, overwrite existing entry. Under Project/Show Table, be sure your corrected protein is the only entry shown.

Perform an energy minimization allowing only the LYS 2 sidechain to move. Use 2 solvent shells around the LYS 2 sidechain(shell #1 at 5.00 angstroms, force constant 200.00, shell #2 at 8.00 angstroms, force constant 500.00).

Calculate the energy of the hybrid protein. Macromodel/Current Energy. Potential AMBER*, Solvent Water, Force Field defined by Structure File, Charges from Force Field, Cutoff Normal. ECalc Energy Listing: Complete.

Analysis/Measurements/Contacts allows you to pick which of the contacts (good, bad, ugly) you want to display. Each type of contact requires a Cut-off Ratio to be filled in (described in further detail below). Good contacts appear as green dashed lines, bad contacts are displayed as orange-yellow dashed lines, and the red dashed lines represent ugly contacts.

C = distance between atom centers/(radius of atom 1 + radius of atom 2)

If C > 1.3	good contact
If 0.89 ≤ C < 1.3	bad contact
If 0.75 ≤ C < 0.89	ugly contact

Set 2

If no ASL, use Set 1.	Calculate intraset contacts.
If ASL,	Calculate all contacts using Set 1 as "from" and Set 2 as "to."

Set 1

If no ASL,	no action.
If ASL	depends on Set 2

ASL = Atomic specification language

eg.	mol. 1	molecule 1
	chain	

Look at the bad contacts. Ftp the hybrid.mmo file to put into Excel to sort for the bad contacts.

7. Perform restricted minimization of the entire hybrid with and without solvent (H_2O). If the presence of solvent does not significantly affect the results, perform all subsequent energy minimizations without solvent.

Perform the minimization holding the backbone atoms (N, C, CA, O, HA) with a force constant of 60 and all sidechain atoms with a force constant of 30. Run minimization manually (bmin) and load the resulting file back into Macromodel to view the minimized structure.

8. Overlay the minimized and original hybrid structures and obtain an RMSD value. Record force constants used, all force field terms (from energy minimization), and RMSD values for each hybrid in a table in Excel.

II. Using Macromodel

The following is a supplement to outline the most commonly used features of the Macromodel software. For further help, consult the online documentation and support manuals accompanying the software Macromodel Interactive Molecular Modeling System Version 7.0[1].

Loading a file into Macromodel

1. Open the macromodel program
2. Go to the **Project** pull-down menu and select **Import Structures**
3. Along the top line of the pop-up menu, highlight "PDB" under where it says Format
4. Highlight "Replace Workspace" and "Import All Structures" underneath the Format box
5. Select "first imported structure" from the pull-down menu next to where it says "Include In Workspace" (Note: if you would like to create one molecule from several PDB files combined, choose "All Imported Structures from this pull-down menu)
6. Click the "Import From" button and select your file from the pop-up menu that appears

Building your own molecule

1. Go to the **Edit** pull-down menu and select **Build**
2. If you wish to build a molecule from existing groups of atoms, left click on the "Fragments" tab and highlight "Place" located just underneath the tab
3. Select the type of atom or atom group you would like from the pull-down menu next to "Fragments"
4. Choose an atom or atom group from the menu of choices below and left click once on the project screen to make it appear
5. If you wish to draw your molecule using individual atoms, select the "Atoms" tab
6. Make sure the "Draw" option is highlighted and select an atom from the few possible choices highlighted in the periodic table below. Note that only a few atoms are available to choose from. Once a basic structure has been built, often using just a carbon atom over and over, each atom can be changed to your liking.
7. To start drawing the structure of the molecule, left click once somewhere in the project screen. Note that a star with a box around it appears. To draw the next atom, left click once somewhere near the first atom. Note that a bond is drawn between them. Continue in this fashion until you have the molecule that you desire. When finished, click once at the end of the last atom you drew. The box will disappear.
8. Now go back and change each atom to the atom you would like it to be by highlighting the "Retype" option next to the "Draw" option that you currently have highlighted. Note that all elements in the periodic table are now available

[1] Mohamadi, F.; Richards, N. G. J.; Guida, W. C.; Liskamp, R.; Lipton, M.; Caufield, C.; Chang, G.; Hendrickson, T.; Still, W. C., "MacroModel-An Integrated Software System for Modeling Organic and Bioorganic Molecules using Molecular Mechanics", *J. Comput. Chem.* **1990**, *11*, 440.

for use. Click on the atom you would like to use and go back to the project screen, left clicking once for every place in your molecule that you would like changed to this new atom.

9. If you have built 2 fragments and would like to connect them to make one molecule, select the "Connect/Fuse" tab.
10. Make sure the "Pick to Define Atom Pairs" option is highlighted toward the bottom of the menu.
11. Go back to the project screen and click on the two atoms you would like to connect/fuse.
12. Now go back to the menu and click either the "Connect" button or the "Fuse" button. Note that connecting the fragments will append one fragment at the end of the other. Fusing the fragments will fuse the end of one fragment into the other one, often changing the shape of the fragments from what you have built.
13. If at any time during your building session you would like to delete one or more atoms, go to the top of the Build window and highlight the "Pick to Delete" option. It doesn't matter if you're under the "Fragments," "Atoms," or "Connect/Fuse" tab; the "Pick to Delete" option can always be highlighted. Once this option has been highlighted, go to the project screen and click on the atoms you would like to delete. Note that "Also delete terminal atoms" option underneath the "Pick to Delete" option. If this is highlighted, all terminal atoms will be deleted as you delete adjacent atoms. If you would like to have single atoms left on the screen after deleting parts of your molecule, do NOT highlight this option.

<u>Manipulating a molecule in Macromodel</u>

1. To rotate the molecule, move the mouse while holding down the middle mouse button
2. If you wish the molecule to rotate around a specific atom, highlight the "Pick to Spot Center" option located at the bottom right of the project screen, then left click on the atom you wish to be the new center point. The molecule will automatically move to put the selected atom at the center of the screen and if the molecule is rotated (hold down middle mouse button), it will now rotate around this new atom. To reset the molecule to make it rotate about its default center point, click the "Fit To Screen" button located at the bottom right of the project screen
3. To resize the molecule, hold down the middle and right mouse buttons simultaneously. Move the mouse forward to enlarge the molecule or backward to shrink the molecule. If you are unsatisfied with the size of the molecule and wish to bring it back to its original size, click the "Fit To Screen" button
4. Use the left mouse button as a pointer to click on specific atoms within the molecule when naming or coloring atoms manually
5. To translate the position of the molecule on the screen, move the mouse while holding down the right mouse button
6. To close any pop-menus, you must left click on the "Hide" button at the bottom left of the menu

Changing the way the molecule is represented on the screen

1. Go to the Display pull-down menu and select Molecular Representation
2. Click on the "Style" tab located at the top of the pop-up menu
3. If you wish to change the appearance of the entire molecule, click on one of the 4 buttons located underneath where it says "Set All To"
4. If you wish to change the appearance of individual atoms or bonds, use the "atoms" and "bonds" tabs located in the middle of the pop-up menu. Select the atom and/or bond representation you desire and make sure the "Pick Atoms to Apply Current Representation" option is highlighted toward the bottom of the screen. Go to the project screen and click on each atom and/or bond you would like to change

Coloring the molecule

1. Go to the **Display** pull-down menu and select **Atom Coloring**
2. If you wish to color atoms individually, select the "Atom Color" tab and then either the "By Palette" or "By Name" tab and select the color you want to use
3. Make sure the "Pick to Apply Current Color" option is highlighted at the bottom of the menu
4. Go to the project screen and left click on each atom you want colored with this color
5. If you wish to color the whole molecule, select the "Color Scheme" tab and select the type of coloring you wish from the menu of choices below. If you click once on each menu choice, a description of that coloring scheme appears in the window above
6. To apply a color scheme, click once on a color scheme from the menu choices, then click the "Apply Scheme to All Atoms" button at the bottom of the screen
7. If you wish to apply a color scheme to specific atoms in the molecule, click once on a color scheme, then highlight the "Pick to Apply Current Scheme" option underneath the color scheme menu. Go to the project screen and left click on each atom you want colored with this scheme

Displaying/Clearing Atom Labels

1. Go to the **Display** pull-down menu and select **Atom Labels**
2. Select the "Composition" tab and highlight the labels you want each atom to have (note that more than one label can be highlighted at the same time).
3. If you would like each label to be listed with its corresponding label heading (ex. atomicnum = 6 instead of just 6), highlight the "Display headings in labels" option at the bottom right of the pop-up window
4. If you wish to label only select atoms by hand, highlight the "Pick to Label Atoms" option at the top of the pop-up window. Otherwise, click the "Label All Atoms" button and every atom in the molecule will be labeled.
5. To clear labels, click the "Clear All Labels" button to clear the labels from the entire molecule, or highlight the "Pick to Clear Labels" option and click on the atom labels you want cleared.
6. To change the font (size and type) of the labels, select the "Appearance" tab in the Atom Labels window

7. To change the color of the labels, select the "Color" tab in the Atom Labels window. Unhighlight the "Color label by atom" option and select the new label color from the palette below.

Changing the Background Color of the Project Screen

1. Go to the **Display** pull-down menu and select **Display Options**
2. Select the "Background" tab, then the "By Palette" tab
3. Click once on the color you wish your background to be (Note that you can select the "By Name" tab instead of the "By Palette" tab to select your new background color by the name of the color you want it to be, however, some of the color names are vague and unhelpful)

Adjusting Bond Orders Within the Molecule

1. Go to the **Edit** menu and select **Bond Properties**
2. Highlight the option according to whether you want to set your own bond order or increment/decrement the bond order of an existing bond. If you choose to set your own bond order, you must choose the type of bond you want from the pull-down menu next to "Bond Order"
3. Go to the project screen and click on the bond you want changed. Note that a green line indicates a zero order bond, a gray line indicates a single bond, a thick gray line indicates a double bond, and a really thick gray line indicates a triple bond.

Displaying and/or Adjusting Bond Angles Within the Molecule

1. Go to the Edit pull-down menu and select Adjust
2. If you wish to adjust a bond length, select the "Distance" tab. If you wish to adjust an angle or a dihedral angle, select the "Angle" or "Dihedral" tab respectively. To display the length/angle, highlight the "Show Markers" and "Define by Picking" options. Go to the project menu and look at the toolbar on the right-hand side has the "Atoms" option highlighted under "Pick States" (Note that you can also choose lengths and angles by highlighting bonds instead of atoms).
3. Click on 2 atoms if selecting a bond length or 3 atoms if selecting a bond angle. Note that an arrow and a number appear on the screen. If you wish only to display the length/angle without adjusting it, unhighlight the "Allow Adjusting" option in the "Adjust" window and Hide the Adjust window. If you wish to adjust the length/angle, move the mouse while holding the middle mouse button down. When you're satisfied with the new length/angle, Hide the Adjust window.
4. If, once the new bond length/angle has been set, you would like to get rid of the numerical labels, go to the bottom of the Adjust window and click the "Delete" button to delete the selected label or "Delete All" to delete all the labels in the molecule.

Adjusting Charges on Atoms, Atom Names, and Residue Numbers
Note that none of these changes will be seen until you display the atom labels for each adjusted atom.

1. Go to the **Edit** pull-down menu and select **Atom Properties**

Adjusting Formal Charge

If you wish to adjust the formal charge on one or more atoms, highlight the "Formal Charge" option under "Select the Atom Properties to Set." Next, highlight the option according to whether you want to set your own formal charge or increment/decrement an existing formal charge. If you choose to set your own formal charge, you must type the value of the new charge in the text box next to "Formal Charge."
Go to the project screen and click on the atoms you want to have new formal charges.

Adjusting Partial Charge

If you wish to adjust the partial charge on one or more atoms, highlight the "Partial Charge" option under "Select the Atom Properties to Set." Type in values for "Charge 1" and "Charge 2" and make sure the "Pick to apply charges" option is highlighted. Note that the value for Charge 1 will be used in molecular mechanics calculations and the value for Charge 2 will be used in GB/SA solvation calculations. Usually, Charge 1 and Charge 2 are set to be the same number. Go to the project screen and click on the atoms you want to have new partial charges.

Adjusting Atom Names

If you wish to change the PDB names, highlight the "PDB Atom Name" option and type a new PDB name into the text box next to "Atom PDB Name." Highlight the "Pick to apply PDB atom name" option. Go to the project screen and click on the atoms you want to change.

If you wish to change the atom names, highlight the "Atom Name" option and select the tab according to whether you want a Unique Name, a Canonical Name, or a Specified Name.

A Unique Name is a computer generated name, combining the element and atom number of each atom, which can only be applied to the whole molecule, not individual atoms. Simply click the "Apply unique name to all atoms" button.

A Canonical Name is a generated using a pair of atom properties, either "element & atom number" or "chain residue number & PDB atom." As with the Unique Name, the Canonical Name can only be applied to the molecule as a whole, however, you get to choose which of the 2 pairs of atom properties you want to use from the pull-down menu next to "Atom Property Pairs." Next, choose the way in which you want the 2 labels to be separated on the screen (ex. comma, semicolon, dash, etc.) and type that into the text box next to "User Specified Separator." Finally, click the "Apply canonical name to all atoms" button.

A Specified Name is a name chosen by you and, unlike the previous 2 naming methods, this naming method is applied to individual atoms. The name can be any length and any combination of capital and lowercase letters, however, the name CANNOT have any spaces in it. Simply type the new name into the text box next to "User Specified

Name" and highlight the "Pick to assign specified atom name" option. Go to the project screen and click on the atoms you want to change.

Adjusting Residue Numbers

If you wish to change residue numbers, highlight the "Residue Properties" option, and type a new residue number into the text box next to "Residue Number." Highlight the "Pick to apply residue number" option. Go to the project screen and click on the atoms you want to change.

Displaying Hydrogens and Lone Pairs of Electrons

1. Go to the **Edit** menu and select **Hydrogen Treatment**
2. Choose the type of atom treatment from the pull-down menu next to "Hadd/Hdel Treatments." Once a treatment has been selected, a description of which kind(s) of force fields can be applied to the hydrogen treatment you've selected. Once you've chosen a hydrogen treatment, click the "Apply current treatment to all atoms" button to apply the treatment to the whole molecule, or highlight the "Pick to apply current treatment" option and click on individual atoms in the project screen. The hydrogens appear white on the screen and the lone pairs are orange.

Clearing (but not deleting) the project

1. In the main project screen, left click the "Clear Workspace" button located in the upper right corner of the screen
2. Click "Yes" when the pop-up menu appears

Displaying a molecule that has been cleared

1. Go to the **Project** pull-down menu and select **Show Table**
2. The pop-up menu that appears is a table of all the files that have been loaded into maestro during this session. Find the file in the "Entry Name" column and click its corresponding box under the "In" column. Note that an X appears in the box. Make sure all other boxes in the "In" column are empty, and click on the "Hide" button to close the menu. If you want multiple molecules to be on the screen at the same time, click the boxes under the "In" column corresponding to each desired file. Note that the files containing these molecules must already have been loaded into the program for this method to work.

Printing the molecule

Note that an image must be printed from one of the IMAC's as the maestro software is set up to print plain text, not images to the printers in the MMLab

1. Go to the **Maestro** pull-down menu and select **Save Image**
2. Type in a name for the file in the text box next to "Filename"
3. Highlight the "JPEG" option next to where it says "Image Format"
4. Click the "Save" button, then click "Hide" to close the menu
5. Using one of the IMAC's in the lab, use Fetch to remotely connect to the Octane computer and transfer your newly-created JPEG file to the macintosh
6. Open a program such as Adobe Photoshop and, once in that program, open your JPEG file

7. Edit the file as desired, then print the file as usual

Saving and converting the PDB file to a Macromodel file

1. Once you have your molecule built and colored as desired, go to the **Project** pull-down menu and select **Export**
2. Along the top of the pop-up menu, highlight the format of the molecule to be saved as "Macromodel"
3. Make sure the "Append" and "Save Graphical Information" boxes underneath are not highlighted
4. Under "Structure Source To Be Exported", highlight "Workspace" if you wish to export the molecule currently in your project window. Highlight "Selected Entries" if you wish to export a molecule that has been loaded into the program but is not currently being displayed in the project window
5. Next to "File(s)", choose "Export All Entries To A Single File" if you only have one molecule loaded into the program or if you wish to export all molecules that have been loaded into the same macromodel file. Choose "Export Each Entry To An Individual File" if you have multiple molecules loaded into the program and wish to export each molecule to its own individual file. If you chose the latter of the 2 choices, you have to pick the way the files are going to be described next to "File Names Are" then describe the files accordingly in the text box next to "File"
6. Click the "Export To" button
7. Choose a directory to export the file to and click "Export" at the bottom of the new pop-up menu

III. Sample Program Output

Unambigously Assigned:

PeakNum	Name	ResNum	AtmNam	Shift	D1Shift	Name	ResNum	AtmNam	Shift	D2Shift	Name	ResNum	AtmNam	Shift	D3Shift	Distance
20	CYS	6	HN	9.201	9.197	VAL	5	HN	9.792	9.788	CYS	6	15N	131.19	131.232	4.56819
21	CYS	6	HN	9.201	9.2	TYR	13	HN	9.574	9.572	CYS	6	15N	131.19	131.214	4.31722
36	ASP	29	HN	9.372	9.369	ASP	29	HN	9.372	9.369	ASP	29	15N	131.67	131.646	0
62	LYS	7	HN	8.891	8.889	ILE	8	HN	9.072	9.067	LYS	7	15N	130.58	130.578	2.72551
73	CYS	6	HN	9.201	9.193	LYS	7	HN	8.891	8.89	CYS	6	15N	131.19	131.119	4.38165
87	LYS	7	HN	8.891	8.889	LYS	7	HN	8.891	8.889	LYS	7	15N	130.58	130.552	0
104	CYS	6	HN	9.201	9.197	GLY	10	HN	7.799	7.793	CYS	6	15N	131.19	131.154	3.97993
106	LYS	7	HN	8.891	8.891	GLY	10	HN	7.799	7.798	LYS	7	15N	130.58	130.63	4.9225
107	LYS	7	HN	8.891	8.893	PHE	49	HN	7.744	7.739	LYS	7	15N	130.58	130.591	4.79926
127	CYS	6	HN	9.201	9.198	PHE	49	HA	5.612	5.606	CYS	6	15N	131.19	131.242	4.77147
128	LYS	7	HN	8.891	8.889	PHE	49	HA	5.612	5.606	LYS	7	15N	130.58	130.553	2.87818
131	CYS	6	HN	9.201	9.197	VAL	5	HA	5.329	5.323	CYS	6	15N	131.19	131.169	2.12192
133	LYS	7	HN	8.891	8.9	VAL	5	HA	5.329	5.322	LYS	7	15N	130.58	130.508	5.47452
140	LYS	7	HN	8.891	8.89	GLU	48	HA	4.659	4.656	LYS	7	15N	130.58	130.627	4.50758
158	CYS	6	HN	9.201	9.198	CYS	6	HB1	2.954	2.952	CYS	6	15N	131.19	131.175	3.00043
162	TRP	4	HE1	9.818	9.812	LYS	51	HA	2.848	2.844	TRP	4	NE1	129.31	129.362	4.76213
171	CYS	6	HN	9.201	9.197	CYS	6	HA	2.753	2.75	CYS	6	15N	131.19	131.172	2.87501
174	LYS	7	HN	8.891	8.889	CYS	6	HA	2.753	2.748	LYS	7	15N	130.58	130.569	2.2696
177	ASP	29	HN	9.372	9.368	PRO	34	HG1	1.982	1.991	ASP	29	15N	131.67	131.644	10.7204
179	LYS	7	HN	8.891	8.885	GLU	48	HB2	2.003	1.998	LYS	7	15N	130.58	130.7	3.67413
190	ASP	29	HN	9.372	9.368	THR	28	HG2*	0.918	0.911	ASP	29	15N	131.67	131.645	19.2383
192	ASP	29	HN	9.372	9.373	VAL	24	HG1*	0.672	0.665	ASP	29	15N	131.67	131.678	19.2383
195	CYS	6	HN	9.201	9.2	ILE	12	HG2*	0.589	0.583	CYS	6	15N	131.19	131.17	7.56526
197	LYS	7	HN	8.891	8.887	ILE	8	HD1*	0.627	0.62	LYS	7	15N	130.58	130.51	3.67413
217	TRP	4	HE1	9.818	9.814	TRP	4	HE1	9.818	9.814	TRP	4	NE1	129.31	129.267	0
236	LEU	52	HN	8.324	8.321	VAL	5	HN	9.792	9.788	LEU	52	15N	126.74	126.711	4.23615
237	ILE	12	HN	7.181	7.177	TYR	13	HN	9.574	9.571	ILE	12	15N	126.71	126.706	4.37118
244	TYR	13	HN	9.574	9.569	TYR	13	HN	9.574	9.57	TYR	13	15N	126.19	126.197	0
362	ASN	25	HN	8.766	8.763	ASN	25	HN	8.766	8.763	ASN	25	15N	127.19	127.157	0
399	LEU	52	HN	8.324	8.324	LYS	3	HN	8.607	8.61	LEU	52	15N	126.74	126.748	3.82736
402	LEU	52	HN	8.324	8.32	LEU	52	HN	8.324	8.321	LEU	52	15N	126.74	126.743	0
416	ASN	14	HN	8.449	8.444	ASN	14	HN	8.449	8.445	ASN	14	15N	126.43	126.413	0
418	TYR	13	HN	9.574	9.569	TRP	4	HN	8.376	8.373	TYR	13	15N	126.19	126.206	2.89162

437 LEU	52 HN	8.324	8.316 GLU	53 HN	8.217	8.217 LEU	52 15N	126.74	126.77	3.91408
446 ASP	54 HN	7.829	7.827 GLU	53 HN	8.217	8.214 ASP	54 15N	125.73	125.742	4.24266
459 TYR	11 HN	9.321	9.317 GLY	10 HN	7.799	7.793 TYR	11 15N	127.93	127.924	2.65673
461 ASN	25 HN	8.766	8.764 ASN	25 HD21	7.586	7.582 ASN	25 15N	127.19	127.137	4.68173
483 ASP	54 HN	7.829	7.826 ASP	54 HN	7.829	7.826 ASP	54 15N	125.73	125.745	0
504 TRP	4 HE1	9.818	9.814 TRP	4 HD1	7.208	7.202 TRP	4 NE1	129.31	129.266	2.56279
505 TRP	4 HE1	9.818	9.812 TRP	4 HH2	7.096	7.093 TRP	4 NE1	129.31	129.202	5.09104
509 TYR	11 HN	9.321	9.318 ILE	12 HN	7.181	7.177 TYR	11 15N	127.93	127.97	4.61825
511 PHE	30 HN	9.033	9.017 TRP	4 HD1	7.208	7.203 PHE	30 15N	127.95	127.776	4.65384
516 ASN	25 HN	8.766	8.764 VAL	24 HN	7.365	7.359 ASN	25 15N	127.19	127.152	4.17573
524 ILE	12 HN	7.181	7.176 ILE	12 HN	7.181	7.177 ILE	12 15N	126.71	126.714	0
538 TYR	13 HN	9.574	9.57 ILE	12 HN	7.181	7.177 TYR	13 15N	126.19	126.249	4.37118
548 LYS	51 HN	7.909	7.904 TRP	4 HH2	7.096	7.09 LYS	51 15N	125.66	125.496	4.99712
558 TYR	13 HN	9.574	9.571 TRP	37 HZ2	6.823	6.815 TYR	13 15N	126.19	126.271	6.77647
565 LYS	51 HN	7.909	7.903 TRP	4 HE3	6.529	6.522 LYS	51 15N	125.66	125.596	3.42575
567 TRP	4 HE1	9.818	9.814 PHE	30 HZ	5.305	5.302 TRP	4 NE1	129.31	129.306	7.83859
568 TYR	11 HN	9.321	9.318 VAL	5 HA	5.329	5.322 TYR	11 15N	127.93	127.899	5.44692
569 PHE	30 HN	9.033	9.027 PHE	30 HZ	5.305	5.302 PHE	30 15N	127.95	127.909	7.90391
570 ILE	12 HN	7.181	7.172 VAL	5 HA	5.329	5.324 ILE	12 15N	126.71	126.741	4.74421
571 TYR	13 HN	9.574	9.57 VAL	5 HA	5.329	5.323 TYR	13 15N	126.19	126.207	3.47637
573 TYR	11 HN	9.321	9.315 CYS	9 HA	4.933	4.925 TYR	11 15N	127.93	127.977	4.58315
577 TYR	13 HN	9.574	9.57 LYS	3 HA	4.903	4.896 TYR	13 15N	126.19	126.286	4.8466
584 TRP	4 HE1	9.818	9.817 ASN	25 HA	4.698	4.695 TRP	4 NE1	129.31	129.278	14.2912
588 PHE	30 HN	9.033	9.036 ASN	25 HA	4.698	4.694 PHE	30 15N	127.95	127.912	11.9097
593 ASN	14 HN	8.449	8.444 ASN	25 HA	4.698	4.694 ASN	14 15N	126.43	126.426	10.4542
599 PHE	30 HN	9.033	9.027 ALA	44 HA	4.31	4.305 PHE	30 15N	127.95	128.28	16.8635
608 LEU	52 HN	8.324	8.319 LEU	52 HA	4.208	4.203 LEU	52 15N	126.74	126.732	2.96156
615 PHE	30 HN	9.033	9.025 THR	28 HB	3.688	3.682 PHE	30 15N	127.95	128.242	6.2576
617 ASN	25 HN	8.766	8.761 PRO	26 HD2	3.556	3.556 ASN	25 15N	127.19	127.218	4.9412
638 LEU	52 HN	8.324	8.321 LYS	51 HA	2.848	2.841 LEU	52 15N	126.74	126.744	2.27477
639 ASN	14 HN	8.449	8.442 TYR	13 HB1	3.115	3.11 ASN	14 15N	126.43	126.424	4.33575
641 TYR	13 HN	9.574	9.569 TYR	13 HB1	3.115	3.11 TYR	13 15N	126.19	126.202	2.87726
644 LYS	51 HN	7.909	7.904 LYS	51 HA	2.848	2.842 LYS	51 15N	125.66	125.664	2.8936
647 TRP	4 HE1	9.818	9.816 PHE	49 HB2	2.608	2.605 TRP	4 NE1	129.31	128.97	7.0195
652 TYR	11 HN	9.321	9.317 CYS	9 HB2	2.436	2.439 TYR	11 15N	127.93	127.882	4.6953
655 LEU	52 HN	8.324	8.326 PHE	49 HB2	2.608	2.598 LEU	52 15N	126.74	126.621	6.96533
663 PHE	30 HN	9.033	9.023 GLU	48 HB2	2.003	1.999 PHE	30 15N	127.95	127.978	15.2522

670 PHE	30 HN	9.033	9.028 GLU	16 HB2	1.741	1.745 PHE	30 15N	127.95	127.939	11.4053
674 ILE	12 HN	7.181	7.177 ILE	12 HG12	1.758	1.769 ILE	12 15N	126.71	126.714	4.6437
679 ASP	54 HN	7.829	7.826 GLU	53 HB1	1.96	1.953 ASP	54 15N	125.73	125.752	2.62774
691 ILE	12 HN	7.181	7.176 ILE	12 HB	1.399	1.392 ILE	12 15N	126.71	126.715	2.39068
695 TYR	13 HN	9.574	9.568 ILE	12 HB	1.399	1.396 TYR	13 15N	126.19	126.214	4.38077
697 ASP	54 HN	7.829	7.826 LEU	52 HB1	1.366	1.366 ASP	54 15N	125.73	125.83	7.49103
699 ASP	54 HN	7.829	7.824 LEU	52 HB2	1.216	1.217 ASP	54 15N	125.73	125.705	6.87329
701 ASN	25 HN	8.766	8.762 THR	28 HG2*	0.918	0.913 ASN	25 15N	127.19	127.157	20.4967
707 ASN	25 HN	8.766	8.763 VAL	24 HG1*	0.672	0.666 ASN	25 15N	127.19	127.154	20.4967
711 ILE	12 HN	7.181	7.175 ILE	12 HG2*	0.589	0.583 ILE	12 15N	126.71	126.706	10.1229
712 ASN	14 HN	8.449	8.443 ILE	12 HG2*	0.589	0.582 ASN	14 15N	126.43	126.356	10.7936
714 TYR	13 HN	9.574	9.569 ILE	12 HG2*	0.589	0.582 TYR	13 15N	126.19	126.198	8.43693
715 ASP	54 HN	7.829	7.824 LEU	52 HD1*	0.728	0.722 ASP	54 15N	125.73	125.784	6.87329
719 LEU	52 HN	8.324	8.322 LYS	51 HG1	0.398	0.387 LEU	52 15N	126.74	126.75	3.03954
720 LEU	52 HN	8.324	8.32 LYS	51 HG2	0.184	0.18 LEU	52 15N	126.74	126.746	3.16391
722 LYS	51 HN	7.909	7.904 LYS	51 HG2	0.184	0.176 LYS	51 15N	125.66	125.654	4.36441
737 PHE	30 HN	9.033	9.026 ILE	33 HD1*	-1.341	-1.349 PHE	30 15N	127.95	128.063	6.52642
761 ILE	8 HN	9.072	9.065 CYS	9 HN	9.165	9.162 ILE	8 15N	121.83	121.861	2.43464
763 ILE	8 HN	9.072	9.066 ILE	8 HN	9.072	9.067 ILE	8 15N	121.83	121.84	0
789 CYS	9 HN	9.165	9.161 CYS	9 HN	9.165	9.162 CYS	9 15N	121.38	121.413	0
791 CYS	9 HN	9.165	9.16 ILE	8 HN	9.072	9.066 CYS	9 15N	121.38	121.419	2.43464
801 ILE	8 HN	9.072	9.067 LYS	7 HN	8.891	8.889 ILE	8 15N	121.83	121.829	2.72551
818 CYS	9 HN	9.165	9.158 LYS	7 HN	8.891	8.888 CYS	9 15N	121.38	121.497	4.55684
824 TRP	37 HN	7.558	7.555 ASP	35 HN	8.247	8.245 TRP	37 15N	124.38	124.409	4.30627
846 TRP	37 HN	7.558	7.554 ASP	36 HN	8.089	8.085 TRP	37 15N	124.38	124.382	2.26216
860 GLU	53 HN	8.217	8.214 GLU	53 HN	8.217	8.214 GLU	53 15N	122.56	122.573	0
929 GLU	53 HN	8.217	8.215 ASP	54 HN	7.829	7.825 GLU	53 15N	122.56	122.584	4.24266
933 ILE	8 HN	9.072	9.067 GLY	10 HN	7.799	7.793 ILE	8 15N	121.83	121.856	3.80447
937 CYS	9 HN	9.165	9.16 GLY	10 HN	7.799	7.793 CYS	9 15N	121.38	121.416	2.1428
968 ILE	33 HN	6.696	6.691 ILE	33 HN	6.696	6.691 ILE	33 15N	124.12	124.127	0
995 TRP	37 HN	7.558	7.553 VAL	38 HN	6.294	6.291 TRP	37 15N	124.38	124.392	4.56634
1010 ILE	8 HN	9.072	9.064 CYS	9 HA	4.933	4.927 ILE	8 15N	121.83	121.726	5.10268
1012 CYS	9 HN	9.165	9.156 CYS	9 HA	4.933	4.929 CYS	9 15N	121.38	121.41	2.96902
1015 ILE	33 HN	6.696	6.698 ASN	25 HA	4.698	4.695 ILE	33 15N	124.12	124.208	10.878
1016 ILE	33 HN	6.696	6.691 ASP	32 HA	4.43	4.426 ILE	33 15N	124.12	124.125	3.35794
1019 LYS	2 HN	8.979	8.973 ASN	25 HA	4.698	4.695 LYS	2 15N	121.55	121.537	13.3502
1037 CYS	9 HN	9.165	9.161 ILE	8 HA	3.959	3.952 CYS	9 15N	121.38	121.401	3.59809

1038 TRP	37 HN	7.558	7.551 PRO	34 HD1	3.659	3.662 TRP	37 15N	124.38	124.612	4.83063
1047 ILE	33 HN	6.696	6.691 ILE	33 HA	3.454	3.448 ILE	33 15N	124.12	124.13	2.8817
1048 ILE	33 HN	6.696	6.692 PRO	34 HD2	3.189	3.183 ILE	33 15N	124.12	124.172	4.73385
1050 ILE	41 HN	8.685	8.676 PRO	40 HD1	3.359	3.357 ILE	41 15N	121.87	121.886	4.01113
1055 GLU	53 HN	8.217	8.212 LYS	51 HA	2.848	2.842 GLU	53 15N	122.56	122.64	4.93917
1056 ILE	41 HN	8.685	8.677 PRO	40 HD2	3.079	3.076 ILE	41 15N	121.87	121.871	3.02593
1057 ILE	8 HN	9.072	9.066 CYS	6 HB1	2.954	2.952 ILE	8 15N	121.83	121.838	4.82246
1060 CYS	9 HN	9.165	9.162 CYS	6 HB1	2.954	2.951 CYS	9 15N	121.38	121.401	4.29294
1061 CYS	9 HN	9.165	9.161 CYS	6 HA	2.753	2.751 CYS	9 15N	121.38	121.39	4.48301
1066 ILE	41 HN	8.685	8.679 ILE	41 HB	2.708	2.703 ILE	41 15N	121.87	121.879	2.56328
1069 ILE	8 HN	9.072	9.067 CYS	6 HA	2.753	2.75 ILE	8 15N	121.83	121.793	3.60556
1075 ILE	33 HN	6.696	6.687 PRO	34 HG1	1.982	1.983 ILE	33 15N	124.12	124.377	7.18852
1079 ILE	41 HN	8.685	8.683 PRO	40 HB1	2.19	2.188 ILE	41 15N	121.87	121.928	3.80538
1089 GLU	53 HN	8.217	8.215 GLU	53 HB1	1.96	1.95 GLU	53 15N	122.56	122.573	3.96496
1105 GLU	53 HN	8.217	8.214 LEU	52 HB2	1.216	1.214 GLU	53 15N	122.56	122.567	4.20811
1118 ILE	33 HN	6.696	6.691 THR	28 HG2*	0.918	0.912 ILE	33 15N	124.12	124.14	16.4826
1119 ILE	33 HN	6.696	6.691 ILE	33 HG11	0.831	0.824 ILE	33 15N	124.12	124.127	3.68976
1122 ILE	41 HN	8.685	8.677 PRO	40 HG2	1.11	1.105 ILE	41 15N	121.87	121.902	4.43236
1127 ILE	33 HN	6.696	6.691 VAL	24 HG1*	0.672	0.667 ILE	33 15N	124.12	124.122	12.2741
1128 GLU	53 HN	8.217	8.214 LEU	52 HD1*	0.728	0.721 GLU	53 15N	122.56	122.573	18.5448
1132 ILE	8 HN	9.072	9.065 ILE	8 HD1*	0.627	0.622 ILE	8 15N	121.83	121.828	11.7987
1135 CYS	9 HN	9.165	9.16 ILE	8 HD1*	0.627	0.621 CYS	9 15N	121.38	121.452	10.7584
1139 TRP	37 HN	7.558	7.554 ILE	33 HG2*	0.076	0.068 TRP	37 15N	124.38	124.384	10.736
1140 ILE	33 HN	6.696	6.691 ILE	33 HB	0.37	0.361 ILE	33 15N	124.12	124.129	2.44725
1141 ILE	33 HN	6.696	6.691 ILE	33 HG2*	0.076	0.071 ILE	33 15N	124.12	124.125	2.44725
1142 GLU	53 HN	8.217	8.219 LYS	51 HG1	0.398	0.39 GLU	53 15N	122.56	122.396	3.78416
1143 ILE	41 HN	8.685	8.682 VAL	38 HG2*	0.237	0.232 ILE	41 15N	121.87	121.897	17.8744
1145 ILE	33 HN	6.696	6.691 ILE	33 HG12	-0.069	-0.079 ILE	33 15N	124.12	124.125	2.45604
1152 ILE	33 HN	6.696	6.691 ILE	33 HD1*	-1.341	-1.347 ILE	33 15N	124.12	124.13	2.45604
1167 TRP	4 HN	8.376	8.373 VAL	5 HN	9.792	9.798 TRP	4 15N	119.19	119.217	4.40217
1170 CYS	9 HN	9.165	9.153 VAL	5 HN	9.792	9.791 CYS	9 15N	121.38	121.235	8.82899
1171 VAL	5 HN	9.792	9.789 VAL	5 HN	9.792	9.788 VAL	5 15N	121.27	121.273	0
1188 TRP	4 HN	8.376	8.37 TYR	13 HN	9.574	9.57 TRP	4 15N	119.19	119.219	2.89162
1221 ASP	21 HN	9.336	9.334 ASP	21 HN	9.336	9.334 ASP	21 15N	120.1	120.09	0
1267 PHE	49 HN	7.744	7.736 GLU	50 HN	9.314	9.309 PHE	49 15N	118.65	118.645	4.55421
1280 CYS	39 HN	8.936	8.932 CYS	39 HN	8.936	8.933 CYS	39 15N	121.11	121.107	0
1292 CYS	42 HN	8.721	8.712 CYS	39 HN	8.936	8.93 CYS	42 15N	120.71	120.986	5.49265

1293 GLU	48 HN	8.413	8.407 CYS	39 HN	8.936	8.934 GLU	48 15N	121.07	121.044	6.47281
1311 CYS	42 HN	8.721	8.715 CYS	42 HN	8.721	8.715 CYS	42 15N	120.71	120.747	0
1324 PHE	49 HN	7.744	7.734 LYS	7 HN	8.891	8.889 PHE	49 15N	118.65	118.543	4.79926
1341 GLU	48 HN	8.413	8.407 GLU	48 HN	8.413	8.408 GLU	48 15N	121.07	121.083	0
1367 LYS	3 HN	8.607	8.605 LYS	3 HN	8.607	8.604 LYS	3 15N	120.48	120.493	0
1379 TRP	4 HN	8.376	8.378 LYS	3 HN	8.607	8.603 TRP	4 15N	119.19	119.208	4.46088
1382 TRP	4 HN	8.376	8.372 TRP	4 HN	8.376	8.373 TRP	4 15N	119.19	119.21	0
1390 PHE	49 HN	7.744	7.738 GLU	48 HN	8.413	8.408 PHE	49 15N	118.65	118.648	2.65834
1404 LYS	46 HN	8.532	8.528 LYS	46 HN	8.532	8.527 LYS	46 15N	118.16	118.163	0
1436 ASP	35 HN	8.247	8.244 ASP	35 HN	8.247	8.244 ASP	35 15N	117.66	117.667	0
1452 ASP	19 HN	8.493	8.488 ASP	19 HN	8.493	8.488 ASP	19 15N	117.29	117.326	0
1461 CYS	39 HN	8.936	8.932 GLY	43 HN	7.847	7.841 CYS	39 15N	121.11	121.105	4.1552
1484 ASP	35 HN	8.247	8.244 ASP	36 HN	8.089	8.084 ASP	35 15N	117.66	117.668	2.88783
1490 GLU	48 HN	8.413	8.407 PHE	49 HN	7.744	7.739 GLU	48 15N	121.07	121.083	2.65834
1502 ASP	21 HN	9.336	9.334 ASN	22 HN	7.647	7.641 ASP	21 15N	120.1	120.098	2.59881
1507 ASN	22 HD22	6.987	6.983 ASN	22 HN	7.647	7.642 ASN	22 ND2	119.6	119.584	3.29805
1524 PHE	49 HN	7.744	7.738 PHE	49 HN	7.744	7.739 PHE	49 15N	118.65	118.646	0
1576 ASP	21 HN	9.336	9.338 VAL	24 HN	7.365	7.359 ASP	21 15N	120.1	120.077	4.79409
1582 TRP	4 HN	8.376	8.371 TRP	4 HD1	7.208	7.202 TRP	4 15N	119.19	119.21	2.86564
1634 VAL	5 HN	9.792	9.789 TRP	4 HE3	6.529	6.523 VAL	5 15N	121.27	121.155	4.46006
1635 CYS	39 HN	8.936	8.933 VAL	38 HN	6.294	6.288 CYS	39 15N	121.11	121.099	4.2582
1651 VAL	5 HN	9.792	9.788 PHE	49 HA	5.612	5.606 VAL	5 15N	121.27	121.262	4.46104
1652 GLU	48 HN	8.413	8.411 PHE	49 HA	5.612	5.603 GLU	48 15N	121.07	121.206	5.03316
1653 CYS	39 HN	8.936	8.932 TRP	37 HH2	5.75	5.743 CYS	39 15N	121.11	121.085	5.19041
1657 PHE	49 HN	7.744	7.737 PHE	49 HA	5.612	5.606 PHE	49 15N	118.65	118.644	2.93521
1659 VAL	5 HN	9.792	9.784 VAL	5 HA	5.329	5.325 VAL	5 15N	121.27	121.271	2.97937
1660 VAL	24 HN	7.365	7.353 ASP	19 HA	5.14	5.139 VAL	24 15N	121.25	121.217	5.00808
1661 ASP	21 HN	9.336	9.335 ASP	19 HA	5.14	5.135 ASP	21 15N	120.1	120.082	3.94662
1663 TRP	4 HN	8.376	8.373 PHE	30 HZ	5.305	5.313 TRP	4 15N	119.19	119.231	8.00325
1667 ASP	19 HN	8.493	8.487 ASP	19 HA	5.14	5.135 ASP	19 15N	117.29	117.317	2.9295
1671 CYS	42 HN	8.721	8.711 CYS	42 HA	4.831	4.825 CYS	42 15N	120.71	120.743	2.92866
1672 LYS	3 HN	8.607	8.603 LYS	3 HA	4.903	4.899 LYS	3 15N	120.48	120.481	2.97047
1680 TRP	4 HN	8.376	8.372 LYS	3 HA	4.903	4.897 TRP	4 15N	119.19	119.214	2.34229
1687 CYS	39 HN	8.936	8.932 VAL	38 HA	4.356	4.351 CYS	39 15N	121.11	121.104	2.19336
1693 ASP	21 HN	9.336	9.34 ASN	25 HA	4.698	4.694 ASP	21 15N	120.1	120.008	6.59616
1696 ASN	22 HD22	6.987	6.997 ASN	25 HA	4.698	4.702 ASN	22 ND2	119.6	119.588	9.5139
1700 PHE	49 HN	7.744	7.738 GLU	48 HA	4.659	4.656 PHE	49 15N	118.65	118.652	3.24001

1704 LYS	46 HN	8.532	8.528 PRO	45 HA	4.641	4.642 LYS	46 15N	118.16	118.165	2.36729
1713 GLU	48 HN	8.413	8.407 LYS	46 HA	4.026	4.019 GLU	48 15N	121.07	121.093	3.83942
1721 PHE	49 HN	7.744	7.739 LYS	46 HA	4.026	4.02 PHE	49 15N	118.65	118.64	3.96086
1724 LYS	46 HN	8.532	8.527 LYS	46 HA	4.026	4.019 LYS	46 15N	118.16	118.166	2.76724
1736 GLU	48 HN	8.413	8.405 PHE	49 HB1	3.645	3.642 GLU	48 15N	121.07	121.135	4.51375
1741 ASP	21 HN	9.336	9.335 PRO	20 HD2	3.812	3.813 ASP	21 15N	120.1	120.12	4.19378
1747 PHE	49 HN	7.744	7.738 PHE	49 HB1	3.645	3.638 PHE	49 15N	118.65	118.647	2.31446
1752 ASP	19 HN	8.493	8.489 PRO	20 HD2	3.812	3.81 ASP	19 15N	117.29	117.339	2.62526
1753 ASP	19 HN	8.493	8.49 PRO	34 HD1	3.659	3.663 ASP	19 15N	117.29	117.371	8.03467
1755 CYS	39 HN	8.936	8.931 PRO	40 HD1	3.359	3.353 CYS	39 15N	121.11	121.11	4.78532
1766 VAL	5 HN	9.792	9.79 LYS	51 HA	2.848	2.842 VAL	5 15N	121.27	121.297	3.95501
1782 TRP	4 HN	8.376	8.372 TYR	13 HB1	3.115	3.109 TRP	4 15N	119.19	119.241	4.72586
1784 TRP	4 HN	8.376	8.38 ASP	19 HB2	2.819	2.827 TRP	4 15N	119.19	119.174	10.713
1786 PHE	49 HN	7.744	7.739 CYS	6 HA	2.753	2.751 PHE	49 15N	118.65	118.673	4.9541
1790 GLU	48 HN	8.413	8.409 PRO	26 HB1	2.395	2.391 GLU	48 15N	121.07	121.064	22.2762
1791 CYS	42 HN	8.721	8.715 ILE	41 HB	2.708	2.702 CYS	42 15N	120.71	120.751	2.41659
1814 ASN	22 HD22	6.987	6.985 PRO	40 HB1	2.19	2.185 ASN	22 ND2	119.6	119.554	3.6106
1817 PHE	49 HN	7.744	7.738 GLU	48 HB2	2.003	1.996 PHE	49 15N	118.65	118.639	4.46536
1841 ASP	35 HN	8.247	8.244 GLU	53 HB1	1.96	1.953 ASP	35 15N	117.66	117.681	22.5941
1853 LYS	46 HN	8.532	8.531 VAL	38 HB	1.455	1.448 LYS	46 15N	118.16	118.188	5.79587
1863 ASP	19 HN	8.493	8.484 THR	28 HG2*	0.918	0.911 ASP	19 15N	117.29	117.34	13.0501
1866 VAL	5 HN	9.792	9.781 ILE	12 HG2*	0.589	0.586 VAL	5 15N	121.27	121.269	13.6501
1871 LYS	3 HN	8.607	8.597 ILE	12 HG2*	0.589	0.584 LYS	3 15N	120.48	120.542	18.3987
1872 LYS	3 HN	8.607	8.606 LEU	52 HD1*	0.728	0.722 LYS	3 15N	120.48	120.432	18.3987
1874 ASN	22 HD22	6.987	6.986 VAL	24 HG2*	0.503	0.496 ASN	22 ND2	119.6	119.623	8.7772
1877 TRP	4 HN	8.376	8.371 ILE	12 HG2*	0.589	0.582 TRP	4 15N	119.19	119.207	14.2
1878 TRP	4 HN	8.376	8.373 LEU	52 HD1*	0.728	0.725 TRP	4 15N	119.19	119.188	14.2
1883 ASP	19 HN	8.493	8.488 VAL	24 HG1*	0.672	0.666 ASP	19 15N	117.29	117.329	13.0501
1885 CYS	39 HN	8.936	8.933 VAL	38 HG2*	0.237	0.231 CYS	39 15N	121.11	121.108	2.52097
1887 CYS	42 HN	8.721	8.711 VAL	38 HG2*	0.237	0.226 CYS	42 15N	120.71	120.793	6.13074
1888 ASP	35 HN	8.247	8.241 ILE	33 HG2*	0.076	0.067 ASP	35 15N	117.66	117.75	11.207
1900 ASP	19 HN	8.493	8.486 ILE	33 HD1*	-1.341	-1.349 ASP	19 15N	117.29	117.457	13.0501
1917 THR	28 HN	6.972	6.964 ASP	29 HN	9.372	9.368 THR	28 15N	115.74	115.725	4.48534
1924 ASN	22 HN	7.647	7.638 ASP	21 HN	9.336	9.334 ASN	22 15N	114.11	114.116	2.59881
1930 ASP	19 HN	8.493	8.488 LYS	2 HN	8.979	8.982 ASP	19 15N	117.29	117.238	11.7193
1931 ASP	19 HN	8.493	8.489 ASN	25 HN	8.766	8.766 ASP	19 15N	117.29	117.255	4.74398
1942 VAL	38 HN	6.294	6.285 CYS	39 HN	8.936	8.933 VAL	38 15N	116.07	116.126	4.2582

1945 THR	28 HN	6.972	6.959 ASN	25 HN	8.766	8.768 THR	28 15N	115.74	115.797	5.28945
1947 ASP	17 HN	7.144	7.135 GLY	27 HN	8.667	8.661 ASP	17 15N	115.49	115.512	4.63747
1974 ASP	17 HN	7.144	7.139 ASN	14 HN	8.449	8.443 ASP	17 15N	115.49	115.464	4.46804
1985 ASP	36 HN	8.089	8.084 ASP	35 HN	8.247	8.244 ASP	36 15N	114.21	114.216	2.88783
1990 ASP	19 HN	8.493	8.487 GLY	18 HN	7.944	7.939 ASP	19 15N	117.29	117.302	4.64471
1996 ASP	17 HN	7.144	7.138 GLY	18 HN	7.944	7.939 ASP	17 15N	115.49	115.494	2.15774
2016 ASP	36 HN	8.089	8.085 ASP	36 HN	8.089	8.085 ASP	36 15N	114.21	114.214	0
2036 GLU	16 HN	7.488	7.483 GLY	18 HN	7.944	7.938 GLU	16 15N	113.61	113.624	3.87581
2084 ASN	22 HN	7.647	7.638 ASN	22 HN	7.647	7.642 ASN	22 15N	114.11	114.122	0
2189 VAL	38 HN	6.294	6.29 VAL	38 HN	6.294	6.291 VAL	38 15N	116.07	116.076	0
2218 ASN	22 HN	7.647	7.632 ASP	19 HA	5.14	5.137 ASN	22 15N	114.11	114.107	4.50708
2222 ASP	32 HN	7.544	7.537 ASP	32 HA	4.43	4.426 ASP	32 15N	116.48	116.483	2.97094
2225 VAL	38 HN	6.294	6.285 PRO	45 HA	4.641	4.641 VAL	38 15N	116.07	116.055	5.59953
2233 GLU	16 HN	7.488	7.481 ASP	17 HA	4.626	4.626 GLU	16 15N	113.61	113.613	5.18941
2251 ASP	32 HN	7.544	7.538 LYS	31 HA	3.611	3.604 ASP	32 15N	116.48	116.511	3.48206
2253 THR	28 HN	6.972	6.965 THR	28 HB	3.688	3.677 THR	28 15N	115.74	115.738	2.47597
2255 ASP	17 HN	7.144	7.139 GLU	16 HA	3.782	3.777 ASP	17 15N	115.49	115.472	3.49487
2256 ASP	17 HN	7.144	7.141 PRO	34 HD1	3.659	3.664 ASP	17 15N	115.49	115.488	13.3929
2263 GLU	16 HN	7.488	7.483 GLU	16 HA	3.782	3.777 GLU	16 15N	113.61	113.614	2.91645
2265 ASP	32 HN	7.544	7.539 ILE	33 HA	3.454	3.446 ASP	32 15N	116.48	116.419	4.88484
2268 ASP	17 HN	7.144	7.139 GLY	18 HA2	3.505	3.495 ASP	17 15N	115.49	115.512	4.9144
2280 THR	28 HN	6.972	6.961 CYS	6 HB2	2.516	2.507 THR	28 15N	115.74	115.737	16.8809
2303 ASN	22 HN	7.647	7.641 PRO	20 HG1	2.094	2.091 ASN	22 15N	114.11	114.175	5.64126
2304 GLU	16 HN	7.488	7.484 PRO	34 HG1	1.982	1.991 GLU	16 15N	113.61	113.682	15.9096
2316 ASP	36 HN	8.089	8.085 GLU	53 HB1	1.96	1.952 ASP	36 15N	114.21	114.226	23.7987
2325 VAL	38 HN	6.294	6.287 VAL	38 HB	1.455	1.448 VAL	38 15N	116.07	116.089	3.88016
2330 ASP	32 HN	7.544	7.539 THR	28 HG2*	0.918	0.912 ASP	32 15N	116.48	116.49	14.9278
2332 THR	28 HN	6.972	6.965 THR	28 HG2*	0.918	0.912 THR	28 15N	115.74	115.747	16.8564
2336 THR	28 HN	6.972	6.964 VAL	24 HG1*	0.672	0.666 THR	28 15N	115.74	115.729	16.8564
2344 VAL	38 HN	6.294	6.29 VAL	38 HG2*	0.237	0.23 VAL	38 15N	116.07	116.077	3.88016
2346 VAL	38 HN	6.294	6.288 ILE	33 HG2*	0.076	0.066 VAL	38 15N	116.07	116.007	3.88016
2347 ASP	36 HN	8.089	8.086 ILE	33 HG2*	0.076	0.07 ASP	36 15N	114.21	114.26	8.94403
2356 ASP	32 HN	7.544	7.537 ILE	33 HD1*	-1.341	-1.346 ASP	32 15N	116.48	116.459	14.9278
2367 GLY	10 HN	7.799	7.793 CYS	9 HN	9.165	9.162 GLY	10 15N	112.56	112.551	2.1428
2368 GLY	10 HN	7.799	7.793 ILE	8 HN	9.072	9.066 GLY	10 15N	112.56	112.538	3.80447
2378 GLY	43 HN	7.847	7.842 CYS	39 HN	8.936	8.932 GLY	43 15N	112.56	112.599	4.1552
2381 GLY	43 HN	7.847	7.841 CYS	42 HN	8.721	8.715 GLY	43 15N	112.56	112.559	2.25635

2523 ASN	25 HD21	7.586	7.582 ASN	25 HD21	7.586	7.582 ASN	25 ND2	112.79	112.771	0
2549 GLY	10 HN	7.799	7.793 GLY	10 HN	7.799	7.793 GLY	10 15N	112.56	112.552	0
2658 ASN	25 HD21	7.586	7.582 ASN	25 HD22	6.916	6.911 ASN	25 ND2	112.79	112.79	1.76709
2734 GLY	10 HN	7.799	7.793 CYS	9 HA	4.933	4.927 GLY	10 15N	112.56	112.568	3.44359
2735 GLY	43 HN	7.847	7.841 CYS	42 HA	4.831	4.825 GLY	43 15N	112.56	112.554	3.49541
2761 GLY	43 HN	7.847	7.842 THR	28 HB	3.688	3.683 GLY	43 15N	112.56	112.46	16.3105
2827 GLY	10 HN	7.799	7.796 ILE	8 HD1*	0.627	0.622 GLY	10 15N	112.56	112.795	18.1626
2836 GLY	43 HN	7.847	7.84 VAL	38 HG2*	0.237	0.23 GLY	43 15N	112.56	112.578	16.3105
2853 GLY	18 HN	7.944	7.94 LYS	2 HN	8.979	8.983 GLY	18 15N	105.3	105.322	8.13568
2907 GLY	18 HN	7.944	7.939 GLU	16 HA	3.782	3.781 GLY	18 15N	105.3	105.348	4.40717
2947 GLY	18 HN	7.944	7.939 GLY	18 HN	7.944	7.939 GLY	18 15N	105.3	105.273	0
3009 GLY	18 HN	7.944	7.939 ASP	17 HA	4.626	4.623 GLY	18 15N	105.3	105.27	3.47955
3016 GLY	18 HN	7.944	7.939 PRO	34 HD1	3.659	3.662 GLY	18 15N	105.3	105.272	11.3162
3045 GLY	18 HN	7.944	7.939 VAL	24 HG1*	0.672	0.665 GLY	18 15N	105.3	105.253	11.3162
3049 ASP	29 HN	9.372	9.368 LYS	2 HN	8.979	8.984 ASP	[illegible]	131.67	131.625	7.40263
3051 ASP	29 HN	9.372	9.368 ASP	29 HB1	2.633	2.635 ASP	[illegible]	131.67	131.625	2.26045
3055 CYS	6 HN	9.201	9.198 GLY	10 HA2	3.586	3.595 CYS	6 15N	131.19	131.125	5.43857
3056 CYS	6 HN	9.201	9.195 PRO	26 HD2	3.556	3.56 CYS	6 15N	131.19	131.125	17.2224
3060 LYS	7 HN	8.891	8.885 CYS	9 HN	9.165	9.158 LYS	7 15N	130.58	130.5	4.55684
3066 TRP	4 HE1	9.818	9.813 ILE	12 HG12	1.758	1.758 TRP	4 NE1	129.31	129.25	9.831
3069 PHE	30 HN	9.033	9.029 CYS	42 HN	8.721	8.722 PHE	30 15N	127.95	128.25	16.8704
3078 PHE	30 HN	9.033	9.03 CYS	42 HB1	3.156	3.157 PHE	30 15N	127.95	128.25	19.6303
3080 TYR	11 HN	9.321	9.318 CYS	9 HN	9.165	9.16 TYR	11 15N	127.93	127.875	3.78724
3085 TYR	11 HN	9.321	9.316 PRO	26 HD2	3.556	3.558 TYR	11 15N	127.93	127.875	18.0163
3088 TYR	11 HN	9.321	9.317 CYS	6 HA	2.753	2.759 TYR	11 15N	127.93	127.875	5.28145
3090 TYR	11 HN	9.321	9.315 ILE	41 HB	2.708	2.704 TYR	11 15N	127.93	127.625	4.47496
3091 TYR	11 HN	9.321	9.317 TYR	11 HB1	3.034	3.043 TYR	11 15N	127.93	127.625	2.66926
3093 TYR	11 HN	9.321	9.311 CYS	9 HA	4.933	4.928 TYR	11 15N	127.93	127.625	4.58315
3094 TYR	11 HN	9.321	9.316 TYR	11 HA	4.142	4.148 TYR	11 15N	127.93	127.625	2.87591
3095 TYR	11 HN	9.321	9.317 LYS	31 HA	3.611	3.604 TYR	11 15N	127.93	127.625	17.0051
3096 TYR	11 HN	9.321	9.316 PRO	26 HD2	3.556	3.561 TYR	11 15N	127.93	127.625	18.0163
3102 ASN	25 HN	8.766	8.761 PRO	26 HD1	3.726	3.724 ASN	25 15N	127.19	127.125	5.0641
3107 LEU	52 HN	8.324	8.319 LEU	52 HD1*	0.728	0.723 LEU	52 15N	126.74	126.75	18.9479
3110 ILE	12 HN	7.181	7.176 ASP	54 HN	7.829	7.835 ILE	12 15N	126.71	126.75	16.8872
3114 ASN	14 HN	8.449	8.443 ASP	54 HB2	2.458	2.453 ASN	14 15N	126.43	126.375	18.9068
3115 ASN	14 HN	8.449	8.443 ASP	35 HB2	2.486	2.497 ASN	14 15N	126.43	126.375	17.319
3116 TYR	13 HN	9.574	9.567 ASN	14 HN	8.449	8.448 TYR	13 15N	126.19	126.25	4.44937

3123 TYR	13 HN	9.574	9.568 LEU	52 HD1*	0.728	0.727 TYR	13 15N	126.19	126.25	4.44937
3124 ASP	54 HN	7.829	7.82 ASP	54 HA	4.246	4.255 ASP	54 15N	125.73	125.75	2.91854
3125 ASP	54 HN	7.829	7.826 GLU	53 HA	4.19	4.186 ASP	54 15N	125.73	125.75	2.36031
3127 ASP	54 HN	7.829	7.827 ASP	54 HB2	2.458	2.453 ASP	54 15N	125.73	125.75	2.44048
3136 TRP	37 HN	7.558	7.555 ILE	41 HB	2.708	2.711 TRP	37 15N	124.38	124.375	13.9916
3140 ILE	33 HN	6.696	6.691 PRO	34 HD1	3.659	3.663 ILE	33 15N	124.12	124.125	5.26582
3141 ILE	33 HN	6.696	6.692 LYS	31 HA	3.611	3.606 ILE	33 15N	124.12	124.125	3.91239
3142 GLU	53 HN	8.217	8.215 LEU	52 HB1	1.366	1.368 GLU	53 15N	122.56	122.625	4.53882
3144 ILE	8 HN	9.072	9.062 ILE	8 HA	3.959	3.955 ILE	8 15N	121.83	121.875	2.93423
3150 ILE	41 HN	8.685	8.668 GLY	43 HN	7.847	7.846 ILE	41 15N	121.87	121.875	3.43051
3153 ILE	41 HN	8.685	8.683 GLU	48 HG2	2.405	2.409 ILE	41 15N	121.87	121.875	10.831
3158 CYS	9 HN	9.165	9.163 LYS	31 HA	3.611	3.61 CYS	9 15N	121.38	121.375	17.1802
3159 CYS	9 HN	9.165	9.162 PRO	26 HD2	3.556	3.562 CYS	9 15N	121.38	121.375	20.7991
3165 VAL	5 HN	9.792	9.786 TRP	4 HN	8.376	8.381 VAL	5 15N	121.27	121.25	4.40217
3166 VAL	5 HN	9.792	9.786 LEU	52 HN	8.324	8.323 VAL	5 15N	121.27	121.25	4.23615
3171 VAL	5 HN	9.792	9.791 LEU	52 HD1*	0.728	0.721 VAL	5 15N	121.27	121.25	4.23615
3178 CYS	39 HN	8.936	8.931 PRO	45 HA	4.641	4.642 CYS	39 15N	121.11	121.125	3.95748
3179 CYS	39 HN	8.936	8.93 ILE	8 HA	3.959	3.953 CYS	39 15N	121.11	121.125	10.1837
3188 CYS	42 HN	8.721	8.716 CYS	42 HB1	3.156	3.153 CYS	42 15N	120.71	120.75	3.76881
3189 CYS	42 HN	8.721	8.715 PRO	40 HD2	3.079	3.079 CYS	42 15N	120.71	120.75	4.99699
3199 ASP	21 HN	9.336	9.334 ASP	32 HB1	2.653	2.66 ASP	21 15N	120.1	120.125	15.0119
3200 ASP	21 HN	9.336	9.34 PRO	20 HG1	2.094	2.091 ASP	21 15N	120.1	120.125	3.29583
3212 PHE	49 HN	7.744	7.739 TRP	4 HE3	6.529	6.526 PHE	49 15N	118.65	118.625	5.20708
3213 PHE	49 HN	7.744	7.738 PHE	49 HB2	2.608	2.605 PHE	49 15N	118.65	118.625	3.56922
3219 LYS	46 HN	8.532	8.53 GLU	16 HB2	1.741	1.737 LYS	46 15N	118.16	118.125	20.6446
3220 ASP	35 HN	8.247	8.241 TYR	11 HA	4.142	4.147 ASP	35 15N	117.66	117.625	19.4704
3223 ASP	35 HN	8.247	8.246 PHE	49 HB2	2.608	2.597 ASP	35 15N	117.66	117.625	13.0773
3226 ASP	19 HN	8.493	8.488 PRO	26 HD1	3.726	3.718 ASP	19 15N	117.29	117.375	5.86499
3229 ASP	19 HN	8.493	8.488 LYS	7 HA	3.892	3.899 ASP	19 15N	117.29	117.375	18.2957
3231 ASP	19 HN	8.493	8.486 PRO	20 HG1	2.094	2.093 ASP	19 15N	117.29	117.375	5.36
3238 THR	28 HN	6.972	6.963 ILE	8 HA	3.959	3.952 THR	28 15N	115.74	115.75	22.7211
3242 ASP	17 HN	7.144	7.134 ASP	17 HA	4.626	4.623 ASP	17 15N	115.49	115.5	2.95138
3245 ASP	17 HN	7.144	7.14 ILE	41 HB	2.708	2.708 ASP	17 15N	115.49	115.5	15.11
3246 ASP	17 HN	7.144	7.139 CYS	6 HA	2.753	2.75 ASP	17 15N	115.49	115.5	14.6866
3248 ASP	17 HN	7.144	7.14 ASP	54 HB2	2.458	2.46 ASP	17 15N	115.49	115.5	20.3522
3252 LYS	31 HN	8.673	8.667 ASP	32 HA	4.43	4.429 LYS	31 15N	114.71	114.75	5.32969
3261 ASP	36 HN	8.089	8.086 CYS	6 HA	2.753	2.754 ASP	36 15N	114.21	114.25	14.6839

3262 ASP	36 HN	8.089	8.085 ILE	41 HB	2.708	2.703 ASP	36 15N	114.21	114.25	16.1706
3263 ASP	36 HN	8.089	8.084 ASP	35 HB2	2.486	2.494 ASP	36 15N	114.21	114.25	4.22992
3265 ASP	36 HN	8.089	8.082 ASP	54 HB2	2.458	2.451 ASP	36 15N	114.21	114.25	27.6589
3269 ASN	22 HN	7.647	7.642 PRO	45 HD1	3.764	3.767 ASN	22 15N	114.11	114.125	16.3965
3270 ASN	22 HN	7.647	7.642 PRO	26 HD1	3.726	3.728 ASN	22 15N	114.11	114.125	9.00217
3276 GLU	16 HN	7.488	7.482 PRO	15 HD2	3.883	3.874 GLU	16 15N	113.61	113.625	4.15441
3285 GLU	16 HN	7.488	7.481 ASP	54 HB2	2.458	2.453 GLU	16 15N	113.61	113.625	18.2176
3287 ASN	25 HD21	7.586	7.582 ASN	25 HN	8.766	8.767 ASN	25 ND2	112.79	112.75	4.68173
3288 ASN	25 HD21	7.586	7.592 ASN	25 HA	4.698	4.698 ASN	25 ND2	112.79	112.75	4.56207
3311 GLY	43 HN	7.847	7.834 ALA	44 HA	4.31	4.307 GLY	43 15N	112.56	112.625	5.16708
3315 GLY	43 HN	7.847	7.835 ALA	44 HA	4.31	4.312 GLY	43 15N	112.56	112.5	5.16708
3317 GLY	10 HN	7.799	7.792 GLY	10 HA2	3.586	3.583 GLY	10 15N	112.56	112.5	2.95708
3319 GLY	43 HN	7.847	7.841 CYS	42 HB1	3.156	3.154 GLY	43 15N	112.56	112.5	4.43875
3324 GLY	10 HN	7.799	7.792 CYS	6 HB1	2.954	2.955 GLY	10 15N	112.56	112.5	4.42697
3325 GLY	43 HN	7.847	7.841 ILE	41 HB	2.708	2.706 GLY	43 15N	112.56	112.5	4.58477
3326 GLY	43 HN	7.847	7.839 CYS	42 HB2	2.421	2.419 GLY	43 15N	112.56	112.5	4.20852
3327 GLY	10 HN	7.799	7.791 ASP	54 HB2	2.458	2.448 GLY	10 15N	112.56	112.5	20.0387
3329 GLY	10 HN	7.799	7.794 CYS	6 HA	2.753	2.757 GLY	10 15N	112.56	112.5	4.66246
3333 GLY	43 HN	7.847	7.839 VAL	38 HB	1.455	1.456 GLY	43 15N	112.56	112.5	4.07141
3338 GLY	43 HN	7.847	7.843 GLY	43 HN	7.847	7.845 GLY	43 15N	112.56	112.5	0
3355 GLY	18 HN	7.944	7.94 ASN	14 HN	8.449	8.442 GLY	18 15N	105.3	105.25	4.40099
3356 GLY	18 HN	7.944	7.939 ASP	19 HN	8.493	8.489 GLY	18 15N	105.3	105.25	4.64471
3358 GLY	18 HN	7.944	7.939 GLY	18 HA2	3.505	3.497 GLY	18 15N	105.3	105.25	2.89992
3360 GLY	18 HN	7.944	7.939 ILE	41 HB	2.708	2.706 GLY	18 15N	105.3	105.25	14.3855
3361 GLY	18 HN	7.944	7.938 CYS	6 HA	2.753	2.746 GLY	18 15N	105.3	105.25	14.1095

Unassigned, No D1 assignment:

PeakNum	D1Shift	Name	ResNum	AtmNam	Shift	D2Shift	Name	ResNum	AtmNam	Shift	D3Shift
2751	7.119	PRO	34	HA	4.168	4.172	ASN	25	ND2	112.79	112.6
3203	9.296	GLU	50	HG1	2.108	2.112	ASP	21	15N	120.1	119.9

Unassigned, No D2 assignment:

PeakNum	D2Shift	Name	ResNum	AtmNam	Shift	D1Shift	Name	ResNum	AtmNam	Shift	D3Shift
4	10.926	TYR	11	HE1	7.029	7.046	ASP	29	15N	131.67	131.6
122	6.403	ASP	29	HN	9.372	9.358	ASP	29	15N	131.67	131.7
161	2.986	TRP	4	HE1	9.818	9.814	TRP	4	NE1	129.31	129.3
199	0.386	TRP	4	HE1	9.818	9.806	TRP	4	NE1	129.31	129.4

215	9.905 TRP	4 HE1	9.818	9.811 TRP	4 NE1	129.31	129.3
451	7.995 LYS	51 HN	7.909	7.902 ASP	54 15N	125.73	125.7
676	1.615 LEU	52 HN	8.324	8.32 LEU	52 15N	126.74	126.7
688	1.272 PHE	30 HN	9.033	9.024 ALA	44 15N	128.28	128.1
721	0.386 LYS	51 HN	7.909	7.904 ASP	54 15N	125.73	125.7
1035	4.112 LYS	2 HN	8.979	8.972 ILE	41 15N	121.87	121.5
1053	2.986 ILE	33 HN	6.696	6.691 TRP	37 15N	124.38	124.1
1099	1.535 TRP	37 HN	7.558	7.563 TRP	37 15N	124.38	124.4
1102	1.243 ILE	33 HN	6.696	6.692 TRP	37 15N	124.38	124.1
1116	1.14 TRP	37 HN	7.558	7.553 TRP	37 15N	124.38	124.4
1154	-1.518 ILE	8 HN	9.072	9.056 ILE	41 15N	121.87	121.9
1156	10.962 ASP	21 HN	9.336	9.353 ASP	21 15N	120.1	120
1569	7.282 GLU	48 HN	8.413	8.406 CYS	9 15N	121.38	121.1
1658	5.731 LYS	46 HN	8.532	8.52 PHE	49 15N	118.65	118.3
1685	4.472 TRP	4 HE1	9.818	9.801 CYS	9 15N	121.38	121.1
1699	4.382 TRP	4 HN	8.376	8.375 TRP	4 15N	119.19	119.1
1816	2.202 PHE	49 HN	7.744	7.74 PHE	49 15N	118.65	118.7
1855	1.542 LYS	46 HN	8.532	8.528 LYS	46 15N	118.16	118.2
1856	1.246 LYS	46 HN	8.532	8.526 LYS	46 15N	118.16	118.2
1861	0.942 LYS	46 HN	8.532	8.529 LYS	46 15N	118.16	118.2
1889	-0.055 ASP	21 HN	9.336	9.337 LYS	3 15N	120.48	120.1
1894	-1.446 GLU	48 HN	8.413	8.408 VAL	5 15N	121.27	121
1901	10.96 TYR	11 HD1	7.312	7.3 ASP	32 15N	116.48	116.2
1902	10.951 TRP	4 HZ2	7.372	7.368 ASP	32 15N	116.48	116.2
1904	10.956 ASP	36 HN	8.089	8.101 LYS	31 15N	114.71	114.4
1908	10.099 VAL	38 HN	6.294	6.289 ASP	32 15N	116.48	116.1
2250	3.992 GLU	16 HN	7.488	7.484 GLU	16 15N	113.61	113.6
2270	2.985 TRP	37 HN	7.558	7.542 ASP	32 15N	116.48	116.5
2274	2.985 ILE	41 HN	8.685	8.67 LYS	31 15N	114.71	114.7
2289	2.596 ASP	36 HN	8.089	8.085 ASP	36 15N	114.21	114.2
2352	-0.958 THR	28 HN	6.972	6.962 VAL	38 15N	116.07	115.9
2800	2.378 LYS	31 HN	8.673	8.662 ASN	14 ND2	112.58	112.3
2818	1.545 GLU	16 HN	7.488	7.48 ASN	25 ND2	112.79	112.6
2823	1.54 LYS	51 HN	7.909	7.903 SER	47 15N	109.53	109.5
2911	2.376 GLY	18 HN	7.944	7.941 GLY	18 15N	105.3	105.3
3058	0.716 CYS	6 HN	9.201	9.199 CYS	6 15N	131.19	131.1
3062	2.578 LYS	7 HN	8.891	8.891 LYS	7 15N	130.58	130.5

3063	1.55 LYS	7 HN	8.891	8.887 LYS	7 15N	130.58	130.5
3064	2.338 TRP	4 HE1	9.818	9.817 TRP	4 NE1	129.31	129.3
3067	0.165 TRP	4 HE1	9.818	9.812 TRP	4 NE1	129.31	129.3
3068	0.206 TRP	4 HE1	9.818	9.814 TRP	4 NE1	129.31	129.3
3073	3.945 PHE	30 HN	9.033	9.026 ALA	44 15N	128.28	128.3
3074	3.994 PHE	30 HN	9.033	9.026 ALA	44 15N	128.28	128.3
3075	3.441 PHE	30 HN	9.033	9.024 ALA	44 15N	128.28	128.3
3076	3.485 PHE	30 HN	9.033	9.025 ALA	44 15N	128.28	128.3
3077	3.524 PHE	30 HN	9.033	9.026 ALA	44 15N	128.28	128.3
3084	3.05 TYR	11 HN	9.321	9.317 PHE	30 15N	127.95	127.9
3087	2.694 TYR	11 HN	9.321	9.316 PHE	30 15N	127.95	127.9
3098	4.716 ASN	25 HN	8.766	8.767 ASN	25 15N	127.19	127.1
3099	4.672 ASN	25 HN	8.766	8.757 ASN	25 15N	127.19	127.1
3101	3.671 ASN	25 HN	8.766	8.761 ASN	25 15N	127.19	127.1
3104	2.694 ASN	25 HN	8.766	8.764 ASN	25 15N	127.19	127.1
3105	1.382 LEU	52 HN	8.324	8.321 LEU	52 15N	126.74	126.8
3118	2.592 TYR	13 HN	9.574	9.562 ASN	14 15N	126.43	126.3
3120	1.771 TYR	13 HN	9.574	9.566 ASN	14 15N	126.43	126.3
3137	2.498 TRP	37 HN	7.558	7.552 TRP	37 15N	124.38	124.4
3138	1.247 TRP	37 HN	7.558	7.555 TRP	37 15N	124.38	124.4
3147	1.247 ILE	8 HN	9.072	9.065 ILE	41 15N	121.87	121.9
3148	1.32 ILE	8 HN	9.072	9.068 ILE	41 15N	121.87	121.9
3163	1.316 CYS	9 HN	9.165	9.158 LYS	2 15N	121.55	121.4
3164	1.26 CYS	9 HN	9.165	9.165 LYS	2 15N	121.55	121.4
3169	1.324 VAL	5 HN	9.792	9.786 LYS	2 15N	121.55	121.3
3180	3.995 CYS	39 HN	8.936	8.934 CYS	9 15N	121.38	121.1
3182	3.484 CYS	39 HN	8.936	8.931 CYS	9 15N	121.38	121.1
3183	3.438 CYS	39 HN	8.936	8.931 CYS	9 15N	121.38	121.1
3184	1.44 CYS	39 HN	8.936	8.931 CYS	9 15N	121.38	121.1
3193	1.621 LYS	3 HN	8.607	8.604 CYS	42 15N	120.71	120.5
3197	1.549 LYS	3 HN	8.607	8.598 CYS	42 15N	120.71	120.5
3202	2.596 GLU	50 HN	9.314	9.298 ASP	21 15N	120.1	119.9
3204	2.588 ASN	22 HD22	6.987	6.985 GLU	50 15N	119.83	119.6
3209	1.615 TRP	4 HN	8.376	8.372 ASN	22 ND2	119.6	119.3
3216	2.265 LYS	46 HN	8.532	8.527 LYS	46 15N	118.16	118.1
3232	2.04 ASP	19 HN	8.493	8.489 ASP	35 15N	117.66	117.4
3237	3.994 TRP	37 HD1	6.984	6.967 VAL	38 15N	116.07	115.8

3241	3.392	THR	28 HN	6.972	6.965	VAL	38 15N	116.07	115.8
3243	3.992	ASP	17 HN	7.144	7.138	THR	28 15N	115.74	115.5
3244	3.94	ASP	17 HN	7.144	7.139	THR	28 15N	115.74	115.5
3256	1.271	ILE	41 HN	8.685	8.673	LYS	31 15N	114.71	114.8
3272	2.59	ASN	22 HN	7.647	7.641	ASP	36 15N	114.21	114.1
3277	3.931	GLU	16 HN	7.488	7.482	GLU	16 15N	113.61	113.6
3278	1.925	GLU	16 HN	7.488	7.483	GLU	16 15N	113.61	113.6
3286	2.498	GLU	16 HN	7.488	7.481	GLU	16 15N	113.61	113.6
3290	2.694	ASN	25 HD21	7.586	7.582	ASN	25 ND2	112.79	112.8
3292	2.69	TRP	4 HZ3	6.924	6.912	ASN	25 ND2	112.79	112.8
3296	3.998	GLU	16 HN	7.488	7.489	ASN	25 ND2	112.79	112.6
3341	4.112	LYS	31 HN	8.673	8.659	ASN	14 ND2	112.58	112.3
3343	3.48	LYS	31 HN	8.673	8.663	ASN	14 ND2	112.58	112.3
3351	2.269	LYS	51 HN	7.909	7.904	SER	47 15N	109.53	109.5

Unassigned, No D3 assignment:

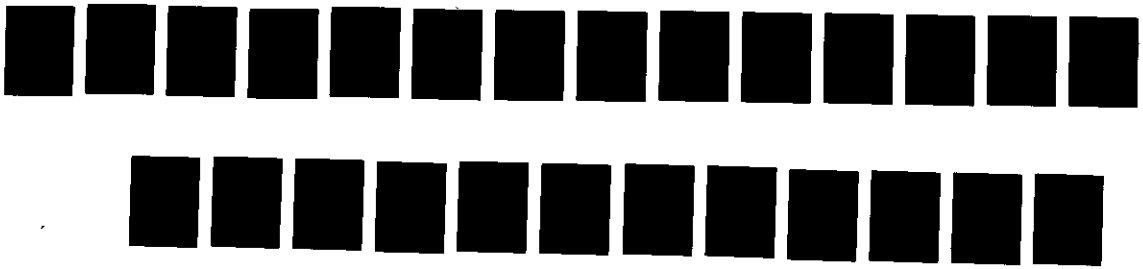
PeakNum	D3Shift	Name	ResNum	AtmNam	Shift	D1Shift	Name	ResNum	AtmNam	Shift	D2Shift

Unassigned, mismatch between D1 and D3 assignment:

PeakNum	Name	ResNum	AtmNam	Shift	D1Shift	Name	ResNum	AtmNam	Shift	D2Shift	Name	ResNum	AtmNam	Shift	D3Shift
237	ILE	12	HN	7.181	7.177	TYR	13	HN	9.574	9.571	LEU	52	15N	126.74	126.706
244	TYR	13	HN	9.574	9.569	TYR	13	HN	9.574	9.57	ASN	14	15N	126.43	126.197
268	PHE	30	HN	9.033	9.027	PHE	30	HN	9.033	9.027	ALA	44	15N	128.28	128.241
298	TYR	11	HN	9.321	9.317	TYR	11	HN	9.321	9.317	ALA	44	15N	128.28	127.925
321	ILE	12	HN	7.181	7.176	TYR	11	HN	9.321	9.317	LEU	52	15N	126.74	126.713
324	TYR	13	HN	9.574	9.568	CYS	6	HN	9.201	9.198	ASN	14	15N	126.43	126.221
416	ASN	14	HN	8.449	8.444	ASN	14	HN	8.449	8.445	LEU	52	15N	126.74	126.413
418	TYR	13	HN	9.574	9.569	TRP	4	HN	8.376	8.373	ASN	14	15N	126.43	126.206
431	PHE	30	HN	9.033	9.027	GLY	43	HN	7.847	7.84	ALA	44	15N	128.28	128.284
452	LYS	51	HN	7.909	7.905	LYS	51	HN	7.909	7.905	ASP	54	15N	125.73	125.674
455	PHE	30	HN	9.033	9.029	PHE	49	HE1	7.458	7.452	ALA	44	15N	128.28	128.33
458	PHE	30	HN	9.033	9.028	ASP	32	HN	7.544	7.538	ALA	44	15N	128.28	128.272
459	TYR	11	HN	9.321	9.317	GLY	10	HN	7.799	7.793	ALA	44	15N	128.28	127.924
462	ASN	14	HN	8.449	8.443	GLU	16	HN	7.488	7.479	LEU	52	15N	126.74	126.431
467	TYR	13	HN	9.574	9.568	PHE	49	HE1	7.458	7.452	ASN	14	15N	126.43	126.231
509	TYR	11	HN	9.321	9.318	ILE	12	HN	7.181	7.177	ALA	44	15N	128.28	127.97
510	TYR	11	HN	9.321	9.317	TYR	11	HD1	7.312	7.305	ALA	44	15N	128.28	127.915

519 ILE	12 HN	7.181	7.173 TYR	11 HD1	7.312	7.307 LEU	52 15N	126.74	126.714
524 ILE	12 HN	7.181	7.176 ILE	12 HN	7.181	7.177 LEU	52 15N	126.74	126.714
536 ASN	14 HN	8.449	8.446 ASP	17 HN	7.144	7.136 LEU	52 15N	126.74	126.406
537 TYR	13 HN	9.574	9.568 TYR	11 HD1	7.312	7.306 ASN	14 15N	126.43	126.212
538 TYR	13 HN	9.574	9.57 ILE	12 HN	7.181	7.177 ASN	14 15N	126.43	126.249
548 LYS	51 HN	7.909	7.904 TRP	4 HH2	7.096	7.09 ASP	54 15N	125.73	125.496
557 ASN	14 HN	8.449	8.447 TYR	11 HE1	7.029	7.022 LEU	52 15N	126.74	126.416
558 TYR	13 HN	9.574	9.571 TRP	37 HZ2	6.823	6.815 ASN	14 15N	126.43	126.271
559 TYR	13 HN	9.574	9.567 TYR	11 HE1	7.029	7.022 ASN	14 15N	126.43	126.157
561 LYS	51 HN	7.909	7.905 TRP	4 HZ3	6.924	6.915 ASP	54 15N	125.73	125.63
565 LYS	51 HN	7.909	7.903 TRP	4 HE3	6.529	6.522 ASP	54 15N	125.73	125.596
568 TYR	11 HN	9.321	9.318 VAL	5 HA	5.329	5.322 PHE	30 15N	127.95	127.899
569 PHE	30 HN	9.033	9.027 PHE	30 HZ	5.305	5.302 ALA	44 15N	128.28	127.909
570 ILE	12 HN	7.181	7.172 VAL	5 HA	5.329	5.324 LEU	52 15N	126.74	126.741
571 TYR	13 HN	9.574	9.57 VAL	5 HA	5.329	5.323 ASN	14 15N	126.43	126.207
572 PHE	30 HN	9.033	9.027 CYS	42 HA	4.831	4.823 ALA	44 15N	128.28	128.344
573 TYR	11 HN	9.321	9.315 CYS	9 HA	4.933	4.925 ALA	44 15N	128.28	127.977
576 ASN	14 HN	8.449	8.441 TRP	4 HA	5.05	5.038 LEU	52 15N	126.74	126.405
577 TYR	13 HN	9.574	9.57 LYS	3 HA	4.903	4.896 ASN	14 15N	126.43	126.286
578 TYR	13 HN	9.574	9.57 TRP	4 HA	5.05	5.039 ASN	14 15N	126.43	126.185
582 LYS	51 HN	7.909	7.904 GLU	50 HA	4.846	4.839 ASP	54 15N	125.73	125.662
583 LYS	51 HN	7.909	7.905 ASN	22 HA	5.061	5.049 ASP	54 15N	125.73	125.477
586 TYR	11 HN	9.321	9.31 ASP	29 HA	4.498	4.491 ALA	44 15N	128.28	128.08
587 PHE	30 HN	9.033	9.028 ASP	29 HA	4.498	4.494 ALA	44 15N	128.28	127.959
588 PHE	30 HN	9.033	9.036 ASN	25 HA	4.698	4.694 ALA	44 15N	128.28	127.912
592 ILE	12 HN	7.181	7.173 ASP	29 HA	4.498	4.488 LEU	52 15N	126.74	126.707
593 ASN	14 HN	8.449	8.444 ASN	25 HA	4.698	4.694 LEU	52 15N	126.74	126.426
594 ASN	14 HN	8.449	8.444 TYR	13 HA	4.396	4.391 LEU	52 15N	126.74	126.413
595 TYR	13 HN	9.574	9.569 ASP	29 HA	4.498	4.488 ASN	14 15N	126.43	126.197
596 TYR	13 HN	9.574	9.566 TYR	13 HA	4.396	4.39 ASN	14 15N	126.43	126.187
597 GLY	43 HN	7.847	7.84 ASN	25 HA	4.698	4.69 ASP	54 15N	125.73	125.789
599 PHE	30 HN	9.033	9.027 ALA	44 HA	4.31	4.305 ALA	44 15N	128.28	128.28
609 ILE	12 HN	7.181	7.176 TYR	11 HA	4.142	4.137 LEU	52 15N	126.74	126.712
611 TYR	13 HN	9.574	9.571 TYR	11 HA	4.142	4.136 LEU	52 15N	126.74	126.384
614 PHE	30 HN	9.033	9.026 PRO	45 HD1	3.764	3.757 ALA	44 15N	128.28	128.286
615 PHE	30 HN	9.033	9.025 THR	28 HB	3.688	3.682 ALA	44 15N	128.28	128.242
625 TYR	11 HN	9.321	9.317 CYS	9 HB1	3.199	3.197 ALA	44 15N	128.28	127.912

629 PHE	30 HN	9.033	9.027 CYS	39 HB1	3.092	3.085 ALA	44 15N	128.28	128.289
630 PHE	30 HN	9.033	9.027 CYS	39 HB2	2.968	2.962 ALA	44 15N	128.28	128.262
637 ILE	12 HN	7.181	7.177 TYR	11 HB1	3.034	3.032 LEU	52 15N	126.74	126.716
639 ASN	14 HN	8.449	8.442 TYR	13 HB1	3.115	3.11 LEU	52 15N	126.74	126.424
640 ASN	14 HN	8.449	8.444 ASN	14 HB1	3.026	3.015 LEU	52 15N	126.74	126.419
641 TYR	13 HN	9.574	9.569 TYR	13 HB1	3.115	3.11 ASN	14 15N	126.43	126.202
642 TYR	13 HN	9.574	9.57 TYR	13 HB2	3.003	2.996 ASN	14 15N	126.43	126.192
644 LYS	51 HN	7.909	7.904 LYS	51 HA	2.848	2.842 ASP	54 15N	125.73	125.664
648 PHE	30 HN	9.033	9.028 CYS	42 HB2	2.421	2.413 ALA	44 15N	128.28	127.997
651 TYR	11 HN	9.321	9.317 ASP	36 HB2	2.521	2.51 ALA	44 15N	128.28	127.924
652 TYR	11 HN	9.321	9.317 CYS	9 HB2	2.436	2.439 PHE	30 15N	127.95	127.882
656 ASN	14 HN	8.449	8.437 TRP	4 HB1	2.617	2.614 ILE	12 15N	126.71	126.355
661 LYS	51 HN	7.909	7.898 ASP	36 HB1	2.733	2.724 ASP	54 15N	125.73	125.658
663 PHE	30 HN	9.033	9.023 GLU	48 HB2	2.003	1.999 ALA	44 15N	128.28	127.978
665 TYR	13 HN	9.574	9.566 ASN	25 HB2	2.359	2.349 ASN	14 15N	126.43	126.095
670 PHE	30 HN	9.033	9.028 GLU	16 HB2	1.741	1.745 ALA	44 15N	128.28	127.939
674 ILE	12 HN	7.181	7.177 ILE	12 HG12	1.758	1.769 LEU	52 15N	126.74	126.714
681 LYS	51 HN	7.909	7.904 GLU	50 HB1	1.835	1.826 ASP	54 15N	125.73	125.662
685 PHE	30 HN	9.033	9.027 ILE	41 HG11	1.414	1.404 ALA	44 15N	128.28	128.278
689 ASP	21 HN	9.336	9.319 LYS	31 HG1	1.202	1.196 ALA	44 15N	128.28	128.032
690 TYR	11 HN	9.321	9.317 ILE	41 HG11	1.414	1.403 ALA	44 15N	128.28	127.907
691 ILE	12 HN	7.181	7.176 ILE	12 HB	1.399	1.392 LEU	52 15N	126.74	126.715
695 TYR	13 HN	9.574	9.568 ILE	12 HB	1.399	1.396 ASN	14 15N	126.43	126.214
697 ASP	54 HN	7.829	7.826 LEU	52 HB1	1.366	1.366 TYR	13 15N	126.19	125.83
700 LYS	51 HN	7.909	7.905 ILE	8 HG11	1.288	1.292 ASP	54 15N	125.73	125.651
702 PHE	30 HN	9.033	9.022 ILE	8 HD1*	0.627	0.622 ALA	44 15N	128.28	128.339
703 PHE	30 HN	9.033	9.025 LYS	51 HB1	0.761	0.753 ALA	44 15N	128.28	128.276
704 PHE	30 HN	9.033	9.03 VAL	38 HG1*	0.508	0.503 ALA	44 15N	128.28	128.28
705 TYR	11 HN	9.321	9.318 ILE	41 HG2*	0.684	0.678 ALA	44 15N	128.28	127.97
706 TYR	11 HN	9.321	9.317 VAL	5 HG1*	0.775	0.766 ALA	44 15N	128.28	127.92
709 ILE	12 HN	7.181	7.175 ILE	12 HD1*	0.742	0.736 LEU	52 15N	126.74	126.703
711 ILE	12 HN	7.181	7.175 ILE	12 HG2*	0.589	0.583 LEU	52 15N	126.74	126.706
712 ASN	14 HN	8.449	8.443 ILE	12 HG2*	0.589	0.582 ILE	12 15N	126.71	126.356
714 TYR	13 HN	9.574	9.569 ILE	12 HG2*	0.589	0.582 ASN	14 15N	126.43	126.198
716 LYS	51 HN	7.909	7.905 LYS	51 HB1	0.761	0.757 ASP	54 15N	125.73	125.67
718 PHE	30 HN	9.033	9.027 VAL	38 HG2*	0.237	0.231 ALA	44 15N	128.28	128.326
722 LYS	51 HN	7.909	7.904 LYS	51 HG2	0.184	0.176 ASP	54 15N	125.73	125.654



737 PHE	30 HN	9.033	9.026 ILE	33 HD1*	-1.341	-1.349 ALA	44 15N	128.28	128.063
761 ILE	8 HN	9.072	9.065 CYS	9 HN	9.165	9.162 ILE	41 15N	121.87	121.861
763 ILE	8 HN	9.072	9.066 ILE	8 HN	9.072	9.067 ILE	41 15N	121.87	121.84
785 TRP	4 HZ2	7.372	7.356 ASP	21 HN	9.336	9.336 LYS	2 15N	121.55	121.372
786 CYS	9 HN	9.165	9.162 TYR	11 HN	9.321	9.315 LYS	2 15N	121.55	121.417
789 CYS	9 HN	9.165	9.161 CYS	9 HN	9.165	9.162 LYS	2 15N	121.55	121.413
791 CYS	9 HN	9.165	9.16 ILE	8 HN	9.072	9.066 LYS	2 15N	121.55	121.419
794 ILE	33 HN	6.696	6.691 LYS	31 HN	8.673	8.671 TRP	37 15N	124.38	124.142
801 ILE	8 HN	9.072	9.067 LYS	7 HN	8.891	8.889 ILE	41 15N	121.87	121.829
818 CYS	9 HN	9.165	9.158 LYS	7 HN	8.891	8.888 ILE	41 15N	121.87	121.497
921 ILE	33 HN	6.696	6.691 ASP	32 HN	7.544	7.539 TRP	37 15N	124.38	124.126
933 ILE	8 HN	9.072	9.067 GLY	10 HN	7.799	7.793 ILE	41 15N	121.87	121.856
937 CYS	9 HN	9.165	9.16 GLY	10 HN	7.799	7.793 LYS	2 15N	121.55	121.416
968 ILE	33 HN	6.696	6.691 ILE	33 HN	6.696	6.691 TRP	37 15N	124.38	124.127
1010 ILE	8 HN	9.072	9.064 CYS	9 HA	4.933	4.927 ILE	41 15N	121.87	121.726
1012 CYS	9 HN	9.165	9.156 CYS	9 HA	4.933	4.929 LYS	2 15N	121.55	121.41
1015 ILE	33 HN	6.696	6.698 ASN	25 HA	4.698	4.695 TRP	37 15N	124.38	124.208
1016 ILE	33 HN	6.696	6.691 ASP	32 HA	4.43	4.426 TRP	37 15N	124.38	124.125
1018 LYS	2 HN	8.979	8.963 ASP	36 HA	4.459	4.449 ILE	41 15N	121.87	121.583
1019 LYS	2 HN	8.979	8.973 ASN	25 HA	4.698	4.695 ILE	41 15N	121.87	121.537
1037 CYS	9 HN	9.165	9.161 ILE	8 HA	3.959	3.952 LYS	2 15N	121.55	121.401
1047 ILE	33 HN	6.696	6.691 ILE	33 HA	3.454	3.448 TRP	37 15N	124.38	124.13
1048 ILE	33 HN	6.696	6.692 PRO	34 HD2	3.189	3.183 TRP	37 15N	124.38	124.172
1051 CYS	9 HN	9.165	9.16 CYS	9 HB1	3.196	3.191 LYS	2 15N	121.55	121.379
1057 ILE	8 HN	9.072	9.066 CYS	6 HB1	2.954	2.952 ILE	41 15N	121.87	121.838
1060 CYS	9 HN	9.165	9.162 CYS	6 HB1	2.954	2.951 LYS	2 15N	121.55	121.401
1061 CYS	9 HN	9.165	9.161 CYS	6 HA	2.753	2.751 LYS	2 15N	121.55	121.39
1062 ILE	33 HN	6.696	6.692 ASP	21 HB1	2.648	2.64 TRP	37 15N	124.38	124.158
1063 ILE	33 HN	6.696	6.695 ASP	29 HB2	2.531	2.52 TRP	37 15N	124.38	124.033
1068 ILE	8 HN	9.072	9.066 ASN	14 HB2	2.479	2.47 ILE	41 15N	121.87	121.846
1069 ILE	8 HN	9.072	9.067 CYS	6 HA	2.753	2.75 ILE	41 15N	121.87	121.793
1075 ILE	33 HN	6.696	6.687 PRO	34 HG1	1.982	1.983 TRP	37 15N	124.38	124.377
1076 ILE	33 HN	6.696	6.691 ASP	32 HB2	2.364	2.356 TRP	37 15N	124.38	124.119
1081 LYS	2 HN	8.979	8.968 GLU	48 HB1	2.219	2.219 ILE	41 15N	121.87	121.52
1082 TRP	4 HZ2	7.372	7.354 PRO	20 HG1	2.094	2.087 LYS	2 15N	121.55	121.347
1092 ILE	8 HN	9.072	9.065 LYS	7 HB1	1.904	1.897 ILE	41 15N	121.87	121.838
1095 ILE	8 HN	9.072	9.066 VAL	24 HB	1.799	1.793 ILE	41 15N	121.87	121.804

1097 VAL	5 HN	9.792	9.787 GLU	50 HB1	1.835	1.828 LYS	2 15N	121.55	121.316
1109 ILE	8 HN	9.072	9.065 ILE	41 HG11	1.414	1.404 ILE	41 15N	121.87	121.784
1118 ILE	33 HN	6.696	6.691 THR	28 HG2*	0.918	0.912 TRP	37 15N	124.38	124.14
1119 ILE	33 HN	6.696	6.691 ILE	33 HG11	0.831	0.824 TRP	37 15N	124.38	124.127
1127 ILE	33 HN	6.696	6.691 VAL	24 HG1*	0.672	0.667 TRP	37 15N	124.38	124.122
1130 ILE	8 HN	9.072	9.065 LYS	51 HB1	0.761	0.751 ILE	41 15N	121.87	121.84
1132 ILE	8 HN	9.072	9.065 ILE	8 HD1*	0.627	0.622 ILE	41 15N	121.87	121.828
1135 CYS	9 HN	9.165	9.16 ILE	8 HD1*	0.627	0.621 LYS	2 15N	121.55	121.452
1137 CYS	9 HN	9.165	9.16 LYS	51 HB1	0.761	0.752 LYS	2 15N	121.55	121.408
1140 ILE	33 HN	6.696	6.691 ILE	33 HB	0.37	0.361 TRP	37 15N	124.38	124.129
1141 ILE	33 HN	6.696	6.691 ILE	33 HG2*	0.076	0.071 TRP	37 15N	124.38	124.125
1145 ILE	33 HN	6.696	6.691 ILE	33 HG12	-0.069	-0.079 TRP	37 15N	124.38	124.125
1152 ILE	33 HN	6.696	6.691 ILE	33 HD1*	-1.341	-1.347 TRP	37 15N	124.38	124.13
1170 CYS	9 HN	9.165	9.153 VAL	5 HN	9.792	9.791 LYS	2 15N	121.55	121.235
1171 VAL	5 HN	9.792	9.789 VAL	5 HN	9.792	9.788 LYS	2 15N	121.55	121.273
1183 TYR	11 HN	9.321	9.31 VAL	5 HN	9.792	9.789 ASP	21 15N	120.1	119.859
1190 VAL	5 HN	9.792	9.79 TYR	11 HN	9.321	9.31 LYS	2 15N	121.55	121.27
1198 CYS	39 HN	8.936	8.932 PHE	30 HN	9.033	9.025 CYS	9 15N	121.38	121.102
1206 CYS	42 HN	8.721	8.715 PHE	30 HN	9.033	9.026 CYS	39 15N	121.11	120.788
1240 ASN	22 HD22	6.987	6.98 ASP	21 HN	9.336	9.325 GLU	50 15N	119.83	119.643
1247 ASN	22 HD22	6.987	6.984 CYS	6 HN	9.201	9.192 GLU	50 15N	119.83	119.603
1253 CYS	6 HN	9.201	9.192 CYS	6 HN	9.201	9.192 GLU	50 15N	119.83	119.531
1276 TRP	4 HZ2	7.372	7.354 ASN	25 HN	8.766	8.762 LYS	2 15N	121.55	121.259
1280 CYS	39 HN	8.936	8.932 CYS	39 HN	8.936	8.933 CYS	9 15N	121.38	121.107
1292 CYS	42 HN	8.721	8.712 CYS	39 HN	8.936	8.93 VAL	5 15N	121.27	120.986
1293 GLU	48 HN	8.413	8.407 CYS	39 HN	8.936	8.934 CYS	9 15N	121.38	121.044
1309 ASP	21 HN	9.336	9.353 CYS	42 HN	8.721	8.717 GLU	48 15N	121.07	120.704
1311 CYS	42 HN	8.721	8.715 CYS	42 HN	8.721	8.715 CYS	39 15N	121.11	120.747
1320 TYR	11 HN	9.321	9.31 LYS	7 HN	8.891	8.888 ASP	21 15N	120.1	119.859
1333 TRP	4 HZ2	7.372	7.358 ASP	19 HN	8.493	8.489 LYS	2 15N	121.55	121.263
1341 GLU	48 HN	8.413	8.407 GLU	48 HN	8.413	8.408 CYS	9 15N	121.38	121.083
1367 LYS	3 HN	8.607	8.605 LYS	3 HN	8.607	8.604 CYS	42 15N	120.71	120.493
1452 ASP	19 HN	8.493	8.488 ASP	19 HN	8.493	8.488 ASP	35 15N	117.66	117.326
1460 GLU	48 HN	8.413	8.407 LYS	51 HN	7.909	7.904 CYS	9 15N	121.38	121.086
1461 CYS	39 HN	8.936	8.932 GLY	43 HN	7.847	7.841 CYS	9 15N	121.38	121.105
1462 CYS	42 HN	8.721	8.715 GLY	43 HN	7.847	7.84 CYS	39 15N	121.11	120.743
1466 TYR	11 HN	9.321	9.309 LYS	51 HN	7.909	7.906 ASP	21 15N	120.1	119.838

1488 TRP	4 HZ2	7.372	7.358 ASN	22 HN	7.647	7.642 LYS	2 15N	121.55	121.249
1489 TRP	4 HZ2	7.372	7.359 PHE	49 HZ	7.54	7.53 LYS	2 15N	121.55	121.254
1490 GLU	48 HN	8.413	8.407 PHE	49 HN	7.744	7.739 CYS	9 15N	121.38	121.083
1491 CYS	39 HN	8.936	8.933 ASP	32 HN	7.544	7.536 CYS	9 15N	121.38	121.113
1494 CYS	39 HN	8.936	8.933 PHE	49 HE1	7.458	7.455 CYS	9 15N	121.38	121.109
1503 ASP	21 HN	9.336	9.335 PHE	49 HZ	7.54	7.53 LYS	3 15N	120.48	120.112
1506 CYS	6 HN	9.201	9.191 ASN	22 HN	7.647	7.642 GLU	50 15N	119.83	119.594
1507 ASN	22 HD22	6.987	6.983 ASN	22 HN	7.647	7.642 GLU	50 15N	119.83	119.584
1554 TRP	4 HZ2	7.372	7.359 TRP	4 HZ2	7.372	7.36 LYS	2 15N	121.55	121.253
1558 GLU	48 HN	8.413	8.416 PHE	49 HE1	7.458	7.448 CYS	9 15N	121.38	121.154
1591 ASP	19 HN	8.493	8.488 TRP	4 HZ2	7.372	7.361 ASP	35 15N	117.66	117.334
1592 TRP	4 HZ2	7.372	7.363 ASN	22 HD22	6.987	6.982 LYS	2 15N	121.55	121.291
1596 TYR	11 HN	9.321	9.311 TRP	4 HZ3	6.924	6.914 ASP	21 15N	120.1	119.933
1598 ASP	21 HN	9.336	9.339 ASN	22 HD22	6.987	6.984 GLU	50 15N	119.83	119.721
1606 CYS	6 HN	9.201	9.191 ASN	22 HD22	6.987	6.984 GLU	50 15N	119.83	119.603
1622 ASN	22 HD22	6.987	6.985 ASN	22 HD22	6.987	6.985 GLU	50 15N	119.83	119.538
1633 CYS	39 HN	8.936	8.934 TRP	37 HE3	6.542	6.536 CYS	9 15N	121.38	121.149
1634 VAL	5 HN	9.792	9.789 TRP	4 HE3	6.529	6.523 CYS	9 15N	121.38	121.155
1635 CYS	39 HN	8.936	8.933 VAL	38 HN	6.294	6.288 CYS	9 15N	121.38	121.099
1638 TYR	11 HN	9.321	9.309 TRP	4 HE3	6.529	6.522 ASP	21 15N	120.1	119.846
1651 VAL	5 HN	9.792	9.788 PHE	49 HA	5.612	5.606 LYS	2 15N	121.55	121.262
1652 GLU	48 HN	8.413	8.411 PHE	49 HA	5.612	5.603 LYS	2 15N	121.55	121.206
1653 CYS	39 HN	8.936	8.932 TRP	37 HH2	5.75	5.743 CYS	9 15N	121.38	121.085
1656 TYR	11 HN	9.321	9.309 PHE	49 HA	5.612	5.606 ASP	21 15N	120.1	119.844
1659 VAL	5 HN	9.792	9.784 VAL	5 HA	5.329	5.325 LYS	2 15N	121.55	121.271
1660 VAL	24 HN	7.365	7.353 ASP	19 HA	5.14	5.139 LYS	2 15N	121.55	121.217
1662 TYR	11 HN	9.321	9.312 VAL	5 HA	5.329	5.327 ASP	21 15N	120.1	119.869
1663 TRP	4 HN	8.376	8.37[illegible] PHE	30 HZ	5.305	5.313 ASN	22 ND2	119.6	119.231
1667 ASP	19 HN	8.493	8.48[illegible] ASP	19 HA	5.14	5.135 ASP	35 15N	117.66	117.317
1668 TRP	4 HZ2	7.372	7.356 ASN	22 HA	5.061	5.054 LYS	2 15N	121.55	121.217
1669 VAL	5 HN	9.792	9.788 TRP	4 HA	5.05	5.045 LYS	2 15N	121.55	121.274
16.0 VAL	5 HN	9.792	9.795 GLU	50 HA	4.846	4.837 LYS	2 15N	121.55	121.183
1671 CYS	42 HN	8.721	8.711 CYS	42 HA	4.831	4.825 CYS	39 15N	121.11	120.743
1672 LYS	3 HN	8.607	8.603 LYS	3 HA	4.903	4.899 CYS	42 15N	120.71	120.481
1674 TYR	11 HN	9.321	9.316 TRP	4 HA	5.05	5.045 ASP	21 15N	120.1	119.955
1675 TYR	11 HN	9.321	9.305 GLU	50 HA	4.846	4.84 ASP	21 15N	120.1	119.841
1677 ASN	22 HD22	6.987	6.984 ASN	22 HA	5.061	5.058 GLU	50 15N	119.83	119.599

1678 CYS	6 HN	9.201	9.193 ASN	22 HA	5.061	5.054 GLU	50 15N	119.83	119.6
1686 GLU	48 HN	8.413	8.406 SER	47 HA	4.363	4.357 CYS	9 15N	121.38	121.093
1687 CYS	39 HN	8.936	8.932 VAL	38 HA	4.356	4.351 CYS	9 15N	121.38	121.104
1690 LYS	3 HN	8.607	8.605 ASP	36 HA	4.459	4.452 CYS	42 15N	120.71	120.495
1696 ASN	22 HD22	6.987	6.997 ASN	25 HA	4.698	4.702 GLU	50 15N	119.83	119.588
1697 CYS	6 HN	9.201	9.2 ASN	25 HA	4.698	4.696 GLU	50 15N	119.83	119.518
1698 TRP	4 HN	8.376	8.372 ASP	29 HA	4.498	4.493 ASN	22 ND2	119.6	119.27
1712 GLU	48 HN	8.413	8.407 ASP	35 HA	4.135	4.125 CYS	9 15N	121.38	121.114
1713 GLU	48 HN	8.413	8.407 LYS	46 HA	4.026	4.019 CYS	9 15N	121.38	121.093
1718 ASP	21 HN	9.336	9.334 PRO	20 HA	4.046	4.039 LYS	3 15N	120.48	120.'05
1719 CYS	6 HN	9.201	9.192 PRO	40 HA	3.978	3.971 GLU	50 15N	119.83	119.594
1720 ASN	22 HD22	6.987	6.985 PRO	40 HA	3.978	3.972 GLU	50 15N	119.83	119.584
1734 GLU	48 HN	8.413	8.406 PRO	20 HD1	3.911	3.932 CYS	9 15N	121.38	121.069
1735 CYS	39 HN	8.936	8.932 CYS	39 HA	3.695	3.688 CYS	9 15N	121.38	121.105
1736 GLU	48 HN	8.413	8.405 PHE	49 HB1	3.645	3.642 CYS	9 15N	121.38	121.135
1737 CYS	42 HN	8.721	8.716 CYS	39 HA	3.695	3.688 CYS	39 15N	121.11	120.864
1741 ASP	21 HN	9.336	9.335 PRO	20 HD2	3.812	3.813 LYS	3 15N	120.48	120.12
1743 TYR	11 HN	9.321	9.311 PHE	49 HB1	3.645	3.638 ASP	21 15N	120.1	119.849
1752 ASP	19 HN	8.493	8.489 PRO	20 HD2	3.812	3.81 ASP	35 15N	117.66	117.339
1753 ASP	19 HN	8.493	8.49 PRO	34 HD1	3.659	3.663 ASP	35 15N	117.66	117.371
1755 CYS	39 HN	8.936	8.931 PRO	40 HD1	3.359	3.353 CYS	9 15N	121.38	121.11
1756 GLU	48 HN	8.413	8.408 PRO	45 HD2	3.509	3.506 CYS	9 15N	121.38	121.062
1766 VAL	5 HN	9.792	9.79 LYS	51 HA	2.848	2.842 LYS	2 15N	121.55	121.297
1767 TRP	4 HZ2	7.372	7.36 ASP	19 HB2	2.819	2.814 LYS	2 15N	121.55	121.236
1768 CYS	39 HN	8.936	8.932 CYS	39 HB1	3.092	3.086 CYS	9 15N	121.38	121.107
1769 CYS	39 HN	8.936	8.932 CYS	39 HB2	2.968	2.96 CYS	9 15N	121.38	121.106
1772 CYS	42 HN	8.721	8.714 CYS	39 HB2	2.968	2.96 GLU	48 15N	121.07	120.722
1774 LYS	3 HN	8.607	8.609 ASP	19 HB2	2.819	2.818 CYS	42 15N	120.71	120.48
1781 CYS	6 HN	9.201	9.191 ASP	19 HB2	2.819	2.812 GLU	50 15N	119.83	119.528
1782 TRP	4 HN	8.376	8.372 TYR	13 HB1	3.115	3.109 ASN	22 ND2	119.6	119.241
1787 ASP	19 HN	8.493	8.489 ASP	19 HB2	2.819	2.813 ASP	35 15N	117.66	117.335
1788 VAL	5 HN	9.792	9.789 TRP	4 HB1	2.617	2.607 LYS	2 15N	121.55	121.265
1789 GLU	48 HN	8.413	8.408 GLU	48 HG1	2.556	2.549 CYS	9 15N	121.38	121.09
1790 GLU	48 HN	8.413	8.409 PRO	26 HB1	2.395	2.391 CYS	9 15N	121.38	121.064
1791 CYS	42 HN	8.721	8.715 ILE	41 HB	2.708	2.702 CYS	39 15N	121.11	120.751
1792 CYS	42 HN	8.721	8.715 CYS	42 HB2	2.421	2.416 CYS	39 15N	121.11	120.74
1796 TYR	11 HN	9.321	9.31 CYS	6 HA	2.753	2.749 ASP	21 15N	120.1	119.859

1797 CYS	6 HN	9.201	9.192 ASP	32 HB1	2.653	2.642 GLU	50 15N	119.83	119.601
1798 ASN	22 HD22	6.987	6.985 ASP	32 HB1	2.653	2.643 GLU	50 15N	119.83	119.576
1804 VAL	5 HN	9.792	9.79 PRO	45 HB1	2.351	2.341 LYS	2 15N	121.55	121.269
1805 TRP	4 HZ2	7.372	7.356 PRO	45 HB2	2.283	2.277 LYS	2 15N	121.55	121.231
1806 GLU	48 HN	8.413	8.408 GLU	48 HB1	2.219	2.213 CYS	9 15N	121.38	121.073
1807 GLU	48 HN	8.413	8.407 GLU	48 HB2	2.003	1.993 CYS	9 15N	121.38	121.083
1809 ASP	21 HN	9.336	9.336 PRO	45 HB2	2.283	2.279 LYS	3 15N	120.48	120.119
1813 CYS	6 HN	9.201	9.192 PRO	40 HB1	2.19	2.185 GLU	50 15N	119.83	119.586
1814 ASN	22 HD22	6.987	6.985 PRO	40 HB1	2.19	2.185 GLU	50 15N	119.83	119.554
1818 LYS	46 HN	8.532	8.528 PRO	45 HG1	2.021	2.014 PHE	49 15N	118.65	118.321
1822 ASP	19 HN	8.493	8.489 PRO	45 HB2	2.283	2.279 ASP	35 15N	117.66	117.482
1823 TRP	4 HZ2	7.372	7.359 VAL	24 HB	1.799	1.793 LYS	2 15N	121.55	121.257
1824 GLU	48 HN	8.413	8.413 ILE	12 HG12	1.758	1.749 LYS	2 15N	121.55	121.287
1825 VAL	5 HN	9.792	9.787 PRO	26 HB2	1.711	1.7 LYS	2 15N	121.55	121.261
1830 TYR	11 HN	9.321	9.309 GLU	50 HB1	1.835	1.826 ASP	21 15N	120.1	119.838
1831 TYR	11 HN	9.321	9.313 VAL	5 HB	1.707	1.697 ASP	21 15N	120.1	119.91
1832 ASN	22 HD22	6.987	6.985 LYS	2 HD1	1.789	1.779 GLU	50 15N	119.83	119.58
1833 CYS	6 HN	9.201	9.191 PRO	40 HG1	1.787	1.776 GLU	50 15N	119.83	119.593
1834 CYS	6 HN	9.201	9.191 PRO	40 HB2	1.642	1.639 GLU	50 15N	119.83	119.569
1835 ASN	22 HD22	6.987	6.985 PRO	40 HB2	1.642	1.639 GLU	50 15N	119.83	119.577
1842 ASP	19 HN	8.493	8.488 VAL	24 HB	1.799	1.793 ASP	35 15N	117.66	117.323
1846 GLU	48 HN	8.413	8.407 ILE	41 HG11	1.414	1.404 CYS	9 15N	121.38	121.052
1847 CYS	42 HN	8.721	8.715 ILE	41 HG11	1.414	1.404 CYS	39 15N	121.11	120.772
1848 LYS	3 HN	8.607	8.602 LYS	3 HG1	1.342	1.349 CYS	42 15N	120.71	120.466
1849 TYR	11 HN	9.321	9.311 LYS	31 HD1	1.566	1.56 ASP	21 15N	120.1	119.895
1850 TYR	11 HN	9.321	9.308 ILE	41 HG11	1.414	1.405 ASP	21 15N	120.1	119.868
1851 TRP	4 HN	8.376	8.372 LYS	3 HG1	1.342	1.343 ASN	22 ND2	119.6	119.243
1863 ASP	19 HN	8.493	8.484 THR	28 HG2*	0.918	0.911 ASP	35 15N	117.66	117.34
1864 VAL	5 HN	9.792	9.788 VAL	5 HG1*	0.775	0.771 LYS	2 15N	121.55	121.276
1865 TRP	4 HZ2	7.372	7.359 VAL	24 HG1*	0.672	0.667 LYS	2 15N	121.55	121.253
1866 VAL	5 HN	9.792	9.781 ILE	12 HG2*	0.589	0.586 LYS	2 15N	121.55	121.269
1867 TRP	4 HZ2	7.372	7.359 VAL	38 HG1*	0.508	0.497 LYS	2 15N	121.55	121.259
1868 CYS	39 HN	8.936	8.932 VAL	38 HG1*	0.508	0.504 CYS	9 15N	121.38	121.101
1870 CYS	42 HN	8.721	8.713 VAL	5 HG1*	0.775	0.767 CYS	39 15N	121.11	120.769
1871 LYS	3 HN	8.607	8.597 ILE	12 HG2*	0.589	0.584 CYS	42 15N	120.71	120.542
1872 LYS	3 HN	8.607	8.606 LEU	52 HD1*	0.728	0.722 CYS	42 15N	120.71	120.432
1873 TYR	11 HN	9.321	9.308 VAL	5 HG1*	0.775	0.771 ASP	21 15N	120.1	119.825

1874 ASN	22 HD22	6.987	6.986 VAL	24 HG2*	0.503	0.496 GLU	50 15N	119.83	119.623
1875 CYS	6 HN	9.201	9.194 VAL	24 HG2*	0.503	0.495 GLU	50 15N	119.83	119.502
1883 ASP	19 HN	8.493	8.488 VAL	24 HG1*	0.672	0.666 ASP	35 15N	117.66	117.329
1885 CYS	39 HN	8.936	8.933 VAL	38 HG2*	0.237	0.231 CYS	9 15N	121.38	121.108
1887 CYS	42 HN	8.721	8.711 VAL	38 HG2*	0.237	0.226 CYS	39 15N	121.11	120.793
1900 ASP	19 HN	8.493	8.486 ILE	33 HD1*	-1.341	-1.349 ASP	35 15N	117.66	117.457
1909 ILE	41 HN	8.685	8.668 TRP	4 HE1	9.818	9.816 LYS	31 15N	114.71	114.642
1915 TRP	37 HN	7.558	7.541 ASP	29 HN	9.372	9.368 ASP	32 15N	116.48	116.481
1917 THR	28 HN	6.972	6.964 ASP	29 HN	9.372	9.368 VAL	38 15N	116.07	115.725
1919 ILE	41 HN	8.685	8.67 PHE	30 HN	9.033	9.028 LYS	31 15N	114.71	114.712
1924 ASN	22 HN	7.647	7.638 ASP	21 HN	9.336	9.334 ASP	36 15N	114.21	114.116
1927 ASN	22 HN	7.647	7.638 CYS	6 HN	9.201	9.192 ASP	36 15N	114.21	114.137
1940 TRP	37 HN	7.558	7.54 LYS	31 HN	8.673	8.67 ASP	32 15N	116.48	116.483
1942 VAL	38 HN	6.294	6.285 CYS	39 HN	8.936	8.933 ASP	32 15N	116.48	116.126
1944 TRP	37 HD1	6.984	6.966 LYS	2 HN	8.979	8.983 VAL	38 15N	116.07	115.728
1945 THR	28 HN	6.972	6.959 ASN	25 HN	8.766	8.768 VAL	38 15N	116.07	115.797
1946 TRP	37 HD1	6.984	6.966 LYS	31 HN	8.673	8.662 VAL	38 15N	116.07	115.741
1947 ASP	17 HN	7.144	7.135 GLY	27 HN	8.667	8.661 THR	28 15N	115.74	115.512
1954 ILE	41 HN	8.685	8.671 LYS	31 HN	8.673	8.67 LYS	31 15N	114.71	114.709
1974 ASP	17 HN	7.144	7.139 ASN	14 HN	8.449	8.443 THR	28 15N	115.74	115.464
1990 ASP	19 HN	8.493	8.487 GLY	18 HN	7.944	7.939 ASP	35 15N	117.66	117.302
1993 TRP	37 HD1	6.984	6.966 GLY	18 HN	7.944	7.94 THR	28 15N	115.74	115.603
1996 ASP	17 HN	7.144	7.138 GLY	18 HN	7.944	7.939 THR	28 15N	115.74	115.494
2058 ASP	17 HN	7.144	7.139 GLU	16 HN	7.488	7.483 THR	28 15N	115.74	115. 93
2063 ILE	41 HN	8.685	8.671 ASP	32 HN	7.544	7.539 LYS	31 15N	114.71	114.715
2084 ASN	22 HN	7.647	7.638 ASN	22 HN	7.647	7.642 ASP	36 15N	114.21	114.122
2090 ASN	22 HN	7.647	7.637 PHE	49 HZ	7.54	7.53 ASP	36 15N	114 21	114.127
2119 ASP	17 HN	7.144	7.141 ASP	17 HN	7.144	7.138 THR	28 15N	115.74	115.491
2137 ASN	22 HN	7.647	7.638 TRP	4 HZ2	7.372	7.36 ASP	36 15N	114.21	114.123
2142 ASP	19 HN	8.493	8.497 TRP	37 HD1	6.984	6.974 ASP	35 15N	117.66	117.293
2147 TRP	37 HN	7.558	7.54 ILE	33 HN	6.696	6.691 ASP	32 15N	116.48	116.489
2149 VAL	38 HN	6.294	6.29 ASN	22 HD22	6.987	6.984 ASP	32 15N	116.48	116.135
2155 TRP	37 HD1	6.984	6.966 THR	28 HN	6.972	6.966 VAL	38 15N	116.07	115.732
2171 ILE	41 HN	8.685	8.671 ILE	33 HN	6.696	6.691 LYS	31 15N	114.71	114.759
2172 ASN	22 HN	7.647	7.643 ASN	22 HD22	6.987	6.983 ASP	36 15N	114.21	114.104
2193 TRP	37 HD1	6.984	6.966 TYR	13 HE1	6.416	6.407 VAL	38 15N	116.07	115.737
2217 ILE	41 HN	8.685	8.671 PHE	30 HZ	5.305	5.302 LYS	31 15N	114.71	114.676

2218 ASN	22 HN	7.647	7.632 ASP	19 HA	5.14	5.137 ASP	36 15N	114.21	114.107
2220 ASN	22 HN	7.647	7.634 ASN	22 HA	5.061	5.059 ASP	36 15N	114.21	114.119
2226 TRP	37 HD1	6.984	6.968 ASN	25 HA	4.698	4.695 VAL	38 15N	116.07	115.72
2229 ILE	41 HN	8.685	8.675 ASN	25 HA	4.698	4.699 LYS	31 15N	114.71	114.719
2230 ILE	41 HN	8.685	8.672 ASP	29 HA	4.498	4.493 LYS	31 15N	114.71	114.646
2242 THR	28 HN	6.972	6.964 VAL	24 HA	4.078	4.068 VAL	38 15N	116.07	115.73
2253 THR	28 HN	6.972	6.965 THR	28 HB	3.688	3.677 VAL	38 15N	116.07	115.738
2255 ASP	17 HN	7.144	7.139 GLU	16 HA	3.782	3.777 THR	28 15N	115.74	115.472
2256 ASP	17 HN	7.144	7.141 PRO	34 HD1	3.659	3.664 THR	28 15N	115.74	115.488
2258 ILE	41 HN	8.685	8.671 LYS	31 HA	3.611	3.605 LYS	31 15N	114.71	114.714
2260 ASN	22 HN	7.647	7.643 PRO	20 HD1	3.911	3.903 ASP	36 15N	114.21	114.027
2266 THR	28 HN	6.972	6.965 PRO	45 HD2	3.509	3.501 VAL	38 15N	116.07	116.04
2268 ASP	17 HN	7.144	7.139 GLY	18 HA2	3.505	3.495 THR	28 15N	115.74	115.512
2269 ASP	19 HN	8.493	8.488 ASP	19 HB1	3.011	3.001 ASP	35 15N	117.66	117.314
2273 ASP	17 HN	7.144	7.137 ASN	14 HB1	3.026	3.018 THR	28 15N	115.74	115.491
2278 TRP	37 HN	7.558	7.541 ASP	29 HB1	2.633	2.635 ASP	32 15N	116.48	116.493
2280 THR	28 HN	6.972	6.961 CYS	6 HB2	2.516	2.507 VAL	38 15N	116.07	115.737
2281 ASN	22 HD22	6.987	6.969 ASP	32 HB2	2.364	2.372 VAL	38 15N	116.07	115.8
2283 ASP	17 HN	7.144	7.137 TRP	4 HB1	2.617	2.615 THR	28 15N	115.74	115.483
2285 ILE	41 HN	8.685	8.671 ASP	29 HB1	2.633	2.624 LYS	31 15N	114.71	114.766
2286 ILE	41 HN	8.685	8.671 ASP	29 HB2	2.531	2.525 LYS	31 15N	114.71	114.741
2294 TRP	37 HN	7.558	7.54 ASP	32 HB2	2.364	2.357 ASP	32 15N	116.48	116.491
2295 TRP	37 HD1	6.984	6.966 PRO	34 HG1	1.982	1.991 VAL	38 15N	116.07	115.705
2301 ASN	22 HN	7.647	7.63 PRO	34 HB1	2.295	2.285 ASP	36 15N	114.21	114.178
2303 ASN	22 HN	7.647	7.641 PRO	20 HG1	2.094	2.091 ASP	36 15N	114.21	114.175
2308 TRP	37 HN	7.558	7.543 LYS	31 HB1	1.712	1.707 ASP	32 15N	116.48	116.453
2309 THR	28 HN	6.972	6.963 PRO	34 HB2	1.85	1.845 VAL	38 15N	116.07	115.716
2310 ASP	17 HN	7.144	7.138 GLU	50 HB1	1.835	1.83 THR	28 15N	115.74	115.506
2311 ASP	17 HN	7.144	7.139 GLU	16 HB2	1.741	1.731 THR	28 15N	115.74	115.5
2314 ILE	41 HN	8.685	8.671 LYS	31 HB1	1.712	1.711 LYS	31 15N	114.71	114.699
2318 ASN	22 HN	7.647	7.634 VAL	24 HB	1.799	1.79 ASP	36 15N	114.21	114.122
2327 ILE	41 HN	8.685	8.671 LYS	31 HD1	1.566	1.567 LYS	31 15N	114.71	114.705
2331 TRP	37 HN	7.558	7.541 ILE	33 HG11	0.831	0.823 ASP	32 15N	116.48	116.488
2332 THR	28 HN	6.972	6.965 THR	28 HG2*	0.918	0.912 VAL	38 15N	116.07	115.747
2333 ILE	41 HN	8.685	8.672 THR	28 HG2*	0.918	0.912 LYS	31 15N	114.71	114.652
2336 THR	28 HN	6.972	6.964 VAL	24 HG1*	0.672	0.666 VAL	38 15N	116.07	115.729
2339 ASN	22 HN	7.647	7.635 VAL	38 HG1*	0.508	0.5 ASP	36 15N	114.21	114.13

2341 TRP	37 HN	7.558	7.543 ILE	33 HB	0.37	0.365 ASP	32 15N	116.48	116.449
2342 TRP	37 HN	7.558	7.54 ILE	33 HG2*	0.076	0.07 ASP	32 15N	116.48	116.371
2349 TRP	37 HN	7.558	7.542 ILE	33 HG12	-0.069	-0.075 ASP	32 15N	116.48	116.35
2359 ILE	41 HN	8.685	8.675 ILE	33 HD1*	-1.341	-1.345 LYS	31 15N	114.71	114.656
2365 GLY	43 HN	7.847	7.841 PHE	30 HN	9.033	9.027 ASN	25 ND2	112.79	112.568
2366 GLY	10 HN	7.799	7.793 TYR	11 HN	9.321	9.317 ASN	25 ND2	112.79	112.55
2367 GLY	10 HN	7.799	7.793 CYS	9 HN	9.165	9.162 ASN	25 ND2	112.79	112.551
2368 GLY	10 HN	7.799	7.793 ILE	8 HN	9.072	9.066 ASN	25 ND2	112.79	112.538
2377 TRP	4 HZ3	6.924	6.913 ASN	25 HN	8.766	8.765 ASN	25 ND2	112.79	112.7[illegible]
2378 GLY	43 HN	7.847	7.842 CYS	39 HN	8.936	8.932 ASN	25 ND2	112.79	112.599
2381 GLY	43 HN	7.847	7.841 CYS	42 HN	8.721	8.715 ASN	25 ND2	112.79	112.559
2389 LYS	31 HN	8.673	8.662 LYS	31 HN	8.673	8.662 ASN	14 ND2	112.58	112.259
2401 GLU	16 HN	7.488	7.48 ASN	14 HN	8.449	8.448 ASN	25 ND2	112.79	112.65
2415 LYS	51 HN	7.909	7.904 LYS	46 HN	8.532	8.528 SER	47 15N	109.53	109.52
2416 LYS	51 HN	7.909	7.904 GLU	48 HN	8.413	8.407 SER	47 15N	109.53	109.525
2440 LYS	31 HN	8.673	8.664 GLY	18 HN	7.944	7.94 ASN	14 ND2	112.58	112.253
2469 LYS	51 HN	7.909	7.904 LYS	51 HN	7.909	7.904 SER	47 15N	109.53	109.52
2494 GLU	16 HN	7.488	7.48 GLU	16 HN	7.488	7.481 ASN	25 ND2	112.79	112.962
2525 TRP	4 HZ3	6.924	6.912 ASN	25 HD21	7.586	7.582 ASN	25 ND2	112.79	112.789
2541 ASP	17 HN	7.144	7.136 GLU	16 HN	7.488	7.479 ASN	25 ND2	112.79	112.573
2549 GLY	10 HN	7.799	7.793 GLY	10 HN	7.799	7.793 ASN	25 ND2	112.79	112.552
2613 GLU	16 HN	7.488	7.479 ASP	17 HN	7.144	7.136 ASN	25 ND2	112.79	112.612
2631 ASP	17 HN	7.144	7.138 ASP	17 HN	7.144	7.136 ASN	25 ND2	112.79	112.508
2633 LYS	31 HN	8.673	8.659 ASP	17 HN	7.144	7.14 ASN	14 ND2	112.58	112.266
2662 TRP	4 HZ3	6.924	6.912 ASN	25 HD22	6.916	6.912 ASN	25 ND2	112.79	112.768
2691 LYS	31 HN	8.673	8.662 THR	28 HN	6.972	6.966 ASN	14 ND2	112.58	112.263
2733 ASP	17 HN	7.144	7.13 ASN	14 HA	5.045	5.037 ASN	25 ND2	112.79	112.561
2734 GLY	10 HN	7.799	7.793 CYS	9 HA	4.933	4.927 ASN	25 ND2	112.79	112.568
2735 GLY	43 HN	7.847	7.841 CYS	42 HA	4.831	4.825 ASN	25 ND2	112.79	112.554
2741 TRP	4 HZ3	6.924	6.92 ASN	25 HA	4.698	4.697 ASN	25 ND2	112.79	112.733
2744 LYS	31 HN	8.673	8.664 ASP	17 HA	4.626	4.622 ASN	14 ND2	112.58	112.266
2755 LYS	31 HN	8.673	8.662 PRO	40 HA	3.978	3.987 ASN	14 ND2	112.58	112.253
2760 GLY	10 HN	7.799	7.79 LYS	7 HA	3.892	3.885 ASN	25 ND2	112.79	112.567
2761 GLY	43 HN	7.847	7.842 THR	28 HB	3.688	3.683 ASN	25 ND2	112.79	112.46
2763 LYS	31 HN	8.673	8.662 GLU	16 HA	3.782	3.778 ASN	14 ND2	112.58	112.269
2765 LYS	31 HN	8.673	8.662 PRO	34 HD1	3.659	3.661 ASN	14 ND2	112.58	112.26
2766 LYS	51 HN	7.909	7.906 GLY	23 HA2	3.75	3.752 SER	47 15N	109.53	109.591

2776 LYS	51 HN	7.909	7.897 PRO	45 HD2	3.509	3.504 SER	47 15N	109.53	109.621
2778 GLU	16 HN	7.488	7.48 ASN	14 HB1	3.026	3.017 ASN	25 ND2	112.79	112.581
2779 GLU	16 HN	7.488	7.479 ASP	19 HB2	2.819	2.816 ASN	25 ND2	112.79	112.582
2780 GLY	43 HN	7.847	7.84 CYS	39 HB1	3.092	3.084 ASN	25 ND2	112.79	112.546
2781 ASP	17 HN	7.144	7.136 ASN	14 HB1	3.026	3.017 ASN	25 ND2	112.79	112.548
2784 ASP	17 HN	7.144	7.136 ASP	19 HB2	2.819	2.816 ASN	25 ND2	112.79	112.554
2789 GLU	16 HN	7.488	7.48 TRP	4 HB1	2.617	2.613 ASN	25 ND2	112.79	113.127
2790 GLU	16 HN	7.488	7.482 ILE	41 HB	2.708	2.702 ASN	25 ND2	112.79	112.857
2804 TRP	4 HZ3	6.924	6.912 ASN	25 HB2	2.359	2.352 ASN	25 ND2	112.79	112.795
2805 LYS	31 HN	8.673	8.659 PRO	34 HG1	1.982	1.989 ASN	14 ND2	112.58	112.305
2811 GLY	10 HN	7.799	7.807 PRO	15 HG1	1.912	1.914 ASN	25 ND2	112.79	112.607
2812 ASP	17 HN	7.144	7.136 GLU	50 HB1	1.835	1.829 ASN	25 ND2	112.79	112.537
2813 ASP	17 HN	7.144	7.137 GLU	16 HB2	1.741	1.73 ASN	25 ND2	112.79	112.503
2814 LYS	31 HN	8.673	8.662 LYS	31 HB1	1.712	1.704 ASN	14 ND2	112.58	112.29
2815 LYS	51 HN	7.909	7.904 LYS	46 HB1	1.862	1.854 SER	47 15N	109.53	109.513
2816 LYS	51 HN	7.909	7.904 GLU	16 HB2	1.741	1.741 SER	47 15N	109.53	109.529
2817 GLU	16 HN	7.488	7.491 LYS	3 HG1	1.342	1.345 ASN	25 ND2	112.79	112.876
2820 ASP	17 HN	7.144	7.135 LYS	3 HD2	1.563	1.553 ASN	25 ND2	112.79	112.566
2825 LYS	51 HN	7.909	7.906 THR	28 HG2*	0.918	0.929 SER	47 15N	109.53	109.524
2827 GLY	10 HN	7.799	7.796 ILE	8 HD1*	0.627	0.622 ASN	25 ND2	112.79	112.795
2830 GLU	16 HN	7.488	7.48 ILE	12 HG2*	0.589	0.585 ASN	25 ND2	112.79	112.545
2831 ASP	17 HN	7.144	7.135 ILE	12 HG2*	0.589	0.584 ASN	25 ND2	112.79	112.533
2832 GLY	43 HN	7.847	7.841 VAL	38 HG1*	0.508	0.505 ASN	25 ND2	112.79	112.535
2833 LYS	31 HN	8.673	8.664 VAL	24 HG1*	0.672	0.669 ASN	14 ND2	112.58	112.259
2835 LYS	51 HN	7.909	7.908 VAL	38 HG1*	0.508	0.504 SER	47 15N	109.53	109.496
2836 GLY	43 HN	7.847	7.84 VAL	38 HG2*	0.237	0.23 ASN	25 ND2	112.79	112.578
2914 LYS	51 HN	7.909	7.9 ILE	41 HG11	1.414	1.404 SER	47 15N	109.53	109.293
2935 ASP	32 HN	7.544	7.535 ASN	22 HD21	9.195	9.189 GLY	23 15N	104.53	104.65
2936 ASP	32 HN	7.544	7.53 ASP	21 HN	9.336	9.334 GLY	23 15N	104.53	104.544
2970 ASP	32 HN	7.544	7.529 ASN	22 HN	7.647	7.641 GLY	23 15N	104.53	104.523
2975 ASP	32 HN	7.544	7.529 PHE	49 HZ	7.54	7.529 GLY	23 15N	104.53	104.521
2991 ASP	32 HN	7.544	7.53 TRP	4 HZ2	7.372	7.36 GLY	23 15N	104.53	104.521
3006 ASP	32 HN	7.544	7.53 ASN	22 HA	5.061	5.057 GLY	23 15N	104.53	104.535
3010 ASP	32 HN	7.544	7.529 TYR	13 HA	4.396	4.392 GLY	23 15N	104.53	104.526
3028 ASP	32 HN	7.544	7.528 ASN	22 HB1	2.93	2.923 GLY	23 15N	104.53	104.527
3034 ASP	32 HN	7.544	7.529 ASP	32 HB1	2.653	2.643 GLY	23 15N	104.53	104.662
3038 ASP	32 HN	7.544	7.528 PRO	45 HB2	2.283	2.276 GLY	23 15N	104.53	104.512

3039 ASP	32 HN	7.544	7.531 PRO	20 HG1	2.094	2.086 GLY	23 15N	104.53	104.412
3042 ASP	32 HN	7.544	7.531 VAL	24 HB	1.799	1.79 GLY	23 15N	104.53	104.437
3044 ASP	32 HN	7.544	7.534 ILE	33 HG11	0.831	0.829 GLY	23 15N	104.53	104.493
3046 ASP	32 HN	7.544	7.53 VAL	38 HG1*	0.508	0.498 GLY	23 15N	104.53	104.536
3069 PHE	30 HN	9.033	9.029 CYS	42 HN	8.721	8.722 ALA	44 15N	128.28	128.25
3070 PHE	30 HN	9.033	9.025 ILE	41 HN	8.685	8.676 ALA	44 15N	128.28	128.25
3078 PHE	30 HN	9.033	9.03 CYS	42 HB1	3.156	3.157 ALA	44 15N	128.28	128.25
3079 PHE	30 HN	9.033	9.025 ASP	36 HB2	2.521	2.517 ALA	44 15N	128.28	128.25
3080 TYR	11 HN	9.321	9.318 CYS	9 HN	9.165	9.16 PHE	30 15N	127.95	127.875
3081 TYR	11 HN	9.321	9.314 CYS	6 HN	9.201	9.197 PHE	30 15N	127.95	127.875
3082 TYR	11 HN	9.321	9.318 TYR	11 HA	4.142	4.142 PHE	30 15N	127.95	127.875
3083 ASP	21 HN	9.336	9.32 CYS	6 HB1	2.954	2.949 PHE	30 15N	127.95	127.875
3085 TYR	11 HN	9.321	9.316 PRO	26 HD2	3.556	3.558 PHE	30 15N	127.95	127.875
3086 ASP	21 HN	9.336	9.319 LYS	31 HA	3.611	3.605 PHE	30 15N	127.95	127.875
3088 TYR	11 HN	9.321	9.317 CYS	6 HA	2.753	2.759 PHE	30 15N	127.95	127.875
3089 ASP	21 HN	9.336	9.319 CYS	6 HA	2.753	2.761 PHE	30 15N	127.95	127.625
3090 TYR	11 HN	9.321	9.315 ILE	41 HB	2.708	2.704 PHE	30 15N	127.95	127.625
3091 TYR	11 HN	9.321	9.317 TYR	11 HB1	3.034	3.043 PHE	30 15N	127.95	127.625
3092 ASP	21 HN	9.336	9.319 CYS	6 HB1	2.954	2.95 PHE	30 15N	127.95	127.625
3093 TYR	11 HN	9.321	9.311 CYS	9 HA	4.933	4.928 PHE	30 15N	127.95	127.625
3094 TYR	11 HN	9.321	9.316 TYR	11 HA	4.142	4.148 PHE	30 15N	127.95	127.625
3095 TYR	11 HN	9.321	9.317 LYS	31 HA	3.611	3.604 PHE	30 15N	127.95	127.625
3096 TYR	11 HN	9.321	9.316 PRO	26 HD2	3.556	3.561 PHE	30 15N	127.95	127.625
3109 ILE	12 HN	7.181	7.175 VAL	5 HG1*	0.775	0.784 LEU	52 15N	126.74	126.75
3110 ILE	12 HN	7.181	7.176 ASP	54 HN	7.829	7.835 LEU	52 15N	126.74	126.75
3111 GLU	48 HN	8.413	8.43 PRO	15 HD1	3.915	3.924 LEU	52 15N	126.74	126.375
3112 ASN	14 HN	8.449	8.435 LYS	7 HA	3.892	3.883 LEU	52 15N	126.74	126.375
3114 ASN	14 HN	8.449	8.443 ASP	54 HB2	2.458	2.453 LEU	52 15N	126.74	126.375
3115 ASN	14 HN	8.449	8.443 ASP	35 HB2	2.486	2.497 LEU	52 15N	126.74	126.375
3116 TYR	13 HN	9.574	9.567 ASN	14 HN	8.449	8.448 ASN	14 15N	126.43	126.25
3117 TYR	13 HN	9.574	9.575 TRP	4 HB1	2.617	2.62 ASN	14 15N	126.43	126.25
3119 TYR	13 HN	9.574	9.57 LYS	31 HB1	1.712	1.703 ASN	14 15N	126.43	126.25
3122 TYR	13 HN	9.574	9.568 VAL	5 HG1*	0.775	0.779 ASN	14 15N	126.43	126.25
3123 TYR	13 HN	9.574	9.568 LEU	52 HD1*	0.728	0.727 ASN	14 15N	126.43	126.25
3128 LYS	51 HN	7.909	7.904 GLU	53 HG2	2.071	2.068 ASP	54 15N	125.73	125.625
3129 LYS	51 HN	7.909	7.909 GLU	50 HG1	2.108	2.117 ASP	54 15N	125.73	125.625
3140 ILE	33 HN	6.696	6.691 PRO	34 HD1	3.659	3.663 TRP	37 15N	124.38	124.125

3141 ILE	33 HN	6.696	6.692 LYS	31 HA	3.611	3.606 TRP	37 15N	124.38	124.125
3144 ILE	8 HN	9.072	9.062 ILE	8 HA	3.959	3.955 ILE	41 15N	121.87	121.875
3145 ILE	8 HN	9.072	9.066 LYS	7 HA	3.892	3.882 ILE	41 15N	121.87	121.875
3154 LYS	2 HN	8.979	8.978 LYS	2 HG1	1.427	1.419 ILE	41 15N	121.87	121.5
3155 CYS	9 HN	9.165	9.164 LYS	7 HA	3.892	3.884 LYS	2 15N	121.55	121.375
3156 CYS	9 HN	9.165	9.169 TYR	11 HA	4.142	4.142 LYS	2 15N	121.55	121.375
3157 CYS	9 HN	9.165	9.162 GLU	53 HA	4.19	4.18 LYS	2 15N	121.55	121.375
3158 CYS	9 HN	9.165	9.163 LYS	31 HA	3.611	3.61 LYS	2 15N	121.55	121.375
3159 CYS	9 HN	9.165	9.162 PRO	26 HD2	3.556	3.562 LYS	2 15N	121.55	121.375
3160 CYS	9 HN	9.165	9.165 TYR	11 HB1	3.034	3.029 LYS	2 15N	121.55	121.375
3161 CYS	9 HN	9.165	9.161 ILE	8 HB	2.475	2.465 LYS	2 15N	121.55	121.375
3162 CYS	9 HN	9.165	9.16 LYS	7 HG2	1.417	1.406 LYS	2 15N	121.55	121.375
3165 VAL	5 HN	9.792	9.786 TRP	4 HN	8.376	8.381 LYS	2 15N	121.55	121.25
3166 VAL	5 HN	9.792	9.786 LEU	52 HN	8.324	8.323 LYS	2 15N	121.55	121.25
3168 TRP	4 HE1	9.818	9.801 LEU	52 HB1	1.366	1.368 LYS	2 15N	121.55	121.25
3170 VAL	5 HN	9.792	9.782 LEU	52 HB2	1.216	1.211 LYS	2 15N	121.55	121.25
3171 VAL	5 HN	9.792	9.791 LEU	52 HD1*	0.728	0.721 LYS	2 15N	121.55	121.25
3172 TRP	4 HZ2	7.372	7.361 PRO	45 HD1	3.764	3.77 LYS	2 15N	121.55	121.25
3173 TRP	4 HZ2	7.372	7.357 PRO	26 HD1	3.726	3.725 LYS	2 15N	121.55	121.25
3174 TRP	4 HZ2	7.372	7.359 THR	28 HA	4.072	4.061 LYS	2 15N	121.55	121.25
3175 TRP	4 HZ2	7.372	7.357 ASN	22 HB1	2.93	2.922 LYS	2 15N	121.55	121.25
3176 TRP	4 HZ2	7.372	7.357 ASP	19 HB1	3.011	3.003 LYS	2 15N	121.55	121.25
3177 GLU	48 HN	8.413	8.414 PRO	34 HB1	2.295	2.285 CYS	9 15N	121.38	121.125
3178 CYS	39 HN	8.936	8.931 PRO	45 HA	4.641	4.642 CYS	9 15N	121.38	121.125
3179 CYS	39 HN	8.936	8.93 ILE	8 HA	3.959	3.953 CYS	9 15N	121.38	121.125
3185 CYS	42 HN	8.721	8.715 PRO	20 HA	4.046	4.041 CYS	39 15N	121.11	120.75
3186 CYS	42 HN	8.721	8.712 GLY	43 HA1	3.975	3.965 CYS	39 15N	121.11	120.75
3187 CYS	42 HN	8.721	8.714 GLY	43 HA2	3.464	3.46 CYS	39 15N	121.11	120.75
3188 CYS	42 HN	8.721	8.716 CYS	42 HB1	3.156	3.153 CYS	39 15N	121.11	120.75
3189 CYS	42 HN	8.721	8.715 PRO	40 HD2	3.079	3.079 CYS	39 15N	121.11	120.75
3190 CYS	42 HN	8.721	8.713 TYR	11 HB1	3.034	3.035 CYS	39 15N	121.11	120.75
3191 CYS	42 HN	8.721	8.715 LYS	31 HG1	1.202	1.191 CYS	39 15N	121.11	120.75
3192 CYS	42 HN	8.721	8.713 ILE	41 HG2*	0.684	0.678 CYS	39 15N	121.11	120.75
3194 LYS	3 HN	8.607	8.602 LYS	31 HB1	1.712	1.702 CYS	42 15N	120.71	120.5
3195 LYS	3 HN	8.607	8.602 LYS	46 HB1	1.862	1.857 CYS	42 15N	120.71	120.5
3196 LYS	3 HN	8.607	8.601 VAL	24 HB	1.799	1.789 CYS	42 15N	120.71	120.5
3198 ASP	21 HN	9.336	9.337 ASN	22 HD22	6.987	6.991 LYS	3 15N	120.48	120.125

3199 ASP	21 HN	9.336	9.334 ASP	32 HB1	2.653	2.66 LYS	3 15N	120.48	120.125
3200 ASP	21 HN	9.336	9.34 PRO	20 HG1	2.094	2.091 LYS	3 15N	120.48	120.125
3201 TYR	11 HN	9.321	9.312 PHE	49 HN	7.744	7.747 ASP	21 15N	120.1	119.875
3205 ASN	22 HD22	6.987	6.986 ASN	22 HB1	2.93	2.927 GLU	50 15N	119.83	119.625
3206 CYS	6 HN	9.201	9.193 ASN	22 HB1	2.93	2.921 GLU	50 15N	119.83	119.625
3207 TRP	4 HN	8.376	8.372 TYR	13 HB2	3.003	2.998 ASN	22 ND2	119.6	119.25
3208 TRP	4 HN	8.376	8.372 LYS	31 HB1	1.712	1.709 ASN	22 ND2	119.6	119.25
3210 TRP	4 HN	8.376	8.371 VAL	5 HG1*	0.775	0.777 ASN	22 ND2	119.6	119.25
3225 ASP	19 HN	8.493	8.488 PRO	45 HD2	3.509	3.498 ASP	35 15N	117.66	117.375
3226 ASP	19 HN	8.493	8.488 PRO	26 HD1	3.726	3.718 ASP	35 15N	117.66	117.375
3228 ASP	19 HN	8.493	8.487 GLY	23 HA1	4.061	4.05 ASP	35 15N	117.66	117.375
3229 ASP	19 HN	8.493	8.488 LYS	7 HA	3.892	3.899 ASP	35 15N	117.66	117.375
3230 ASP	19 HN	8.493	8.49 PRO	40 HA	3.978	3.967 ASP	35 15N	117.66	117.375
3231 ASP	19 HN	8.493	8.486 PRO	20 HG1	2.094	2.093 ASP	35 15N	117.66	117.375
3233 ASP	19 HN	8.493	8.486 VAL	38 HG1*	0.508	0.498 ASP	35 15N	117.66	117.375
3238 THR	28 HN	6.972	6.963 ILE	8 HA	3.959	3.952 VAL	38 15N	116.07	115.75
3240 TRP	37 HD1	6.984	6.966 PRO	40 HD1	3.359	3.351 VAL	38 15N	116.07	115.75
3242 ASP	17 HN	7.144	7.134 ASP	17 HA	4.626	4.623 THR	28 15N	115.74	115.5
3245 ASP	17 HN	7.144	7.14 ILE	41 HB	2.708	2.708 THR	28 15N	115.74	115.5
3246 ASP	17 HN	7.144	7.139 CYS	6 HA	2.753	2.75 THR	28 15N	115.74	115.5
3248 ASP	17 HN	7.144	7.14 ASP	54 HB2	2.458	2.46 THR	28 15N	115.74	115.5
3249 ASP	17 HN	7.144	7.14 ASP	35 HB2	2.486	2.488 THR	28 15N	115.74	115.5
3250 ASP	17 HN	7.144	7.129 GLU	53 HG1	2.161	2.156 THR	28 15N	115.74	115.5
3251 ASP	17 HN	7.144	7.132 GLU	48 HB1	2.219	2.212 THR	28 15N	115.74	115.5
3253 ILE	41 HN	8.685	8.67 CYS	42 HB2	2.421	2.414 LYS	31 15N	114.71	114.75
3254 ILE	41 HN	8.685	8.669 ASP	32 HB2	2.364	2.357 LYS	31 15N	114.71	114.75
3255 ILE	41 HN	8.685	8.67 LYS	31 HG1	1.202	1.202 LYS	31 15N	114.71	114.75
3267 ASN	22 HN	7.647	7.638 TYR	13 HA	4.396	4.394 ASP	36 15N	114.21	114.125
3268 ASN	22 HN	7.647	7.642 PRO	20 HA	4.046	4.04 ASP	36 15N	114.21	114.125
3269 ASN	22 HN	7.647	7.642 PRO	45 HD1	3.764	3.767 ASP	36 15N	114.21	114.125
3270 ASN	22 HN	7.647	7.642 PRO	26 HD1	3.726	3.728 ASP	36 15N	114.21	114.125
3271 ASN	22 HN	7.647	7.641 ASP	32 HB1	2.653	2.644 ASP	36 15N	114.21	114.125
3273 ASN	22 HN	7.647	7.643 ASN	22 HB1	2.93	2.924 ASP	36 15N	114.21	114.125
3291 TRP	4 HZ3	6.924	6.912 ASP	32 HB1	2.653	2.649 ASN	25 ND2	112.79	112.75
3293 GLU	16 HN	7.488	7.478 GLU	16 HN	7.488	7.485 ASN	25 ND2	112.79	112.625
3298 GLU	16 HN	7.488	7.477 ASP	29 HB1	2.633	2.624 ASN	25 ND2	112.79	112.625
3299 GLU	16 HN	7.488	7.482 ASN	14 HA	5.045	5.037 ASN	25 ND2	112.79	112.625

3300 GLU	16 HN	7.488	7.482 GLU	16 HA	3.782	3.775 ASN	25 ND2	112.79	112.625
3301 GLU	16 HN	7.488	7.482 LYS	7 HA	3.892	3.894 ASN	25 ND2	112.79	112.625
3303 GLU	16 HN	7.488	7.48 ASP	54 HB2	2.458	2.453 ASN	25 ND2	112.79	112.625
3304 GLU	16 HN	7.488	7.48 ASP	35 HB2	2.486	2.497 ASN	25 ND2	112.79	112.625
3305 GLU	16 HN	7.488	7.48 GLU	16 HB2	1.741	1.731 ASN	25 ND2	112.79	112.625
3306 GLU	16 HN	7.488	7.479 GLU	50 HB1	1.835	1.833 ASN	25 ND2	112.79	112.625
3307 GLU	16 HN	7.488	7.483 GLU	16 HG1	2.215	2.206 ASN	25 ND2	112.79	112.625
3309 ASP	17 HN	7.144	7.133 ASP	54 HB2	2.458	2.453 ASN	25 ND2	112.79	112.625
3310 ASP	17 HN	7.144	7.136 ASP	35 HB2	2.486	2.495 ASN	25 ND2	112.79	112.625
3311 GLY	43 HN	7.847	7.834 ALA	44 HA	4.31	4.307 ASN	25 ND2	112.79	112.625
3312 GLY	43 HN	7.847	7.838 SER	47 HA	4.363	4.352 ASN	25 ND2	112.79	112.625
3313 GLY	10 HN	7.799	7.786 PRO	34 HA	4.168	4.161 ASN	25 ND2	112.79	112.5
3314 GLY	43 HN	7.847	7.837 SER	47 HA	4.363	4.357 ASN	25 ND2	112.79	112.5
3315 GLY	43 HN	7.847	7.835 ALA	44 HA	4.31	4.312 ASN	25 ND2	112.79	112.5
3316 GLY	43 HN	7.847	7.845 PRO	40 HA	3.978	3.973 ASN	25 ND2	112.79	112.5
3317 GLY	10 HN	7.799	7.792 GLY	10 HA2	3.586	3.583 ASN	25 ND2	112.79	112.5
3318 GLY	43 HN	7.847	7.838 GLY	43 HA2	3.464	3.459 ASN	25 ND2	112.79	112.5
3319 GLY	43 HN	7.847	7.841 CYS	42 HB1	3.156	3.154 ASN	25 ND2	112.79	112.5
3320 GLY	10 HN	7.799	7.794 CYS	9 HB1	3.199	3.194 ASN	25 ND2	112.79	112.5
3321 GLY	10 HN	7.799	7.792 TYR	11 HB1	3.034	3.034 ASN	25 ND2	112.79	112.5
3323 GLY	43 HN	7.847	7.844 CYS	39 HB2	2.968	2.958 ASN	25 ND2	112.79	112.5
3324 GLY	10 HN	7.799	7.792 CYS	6 HB1	2.954	2.955 ASN	25 ND2	112.79	112.5
3325 GLY	43 HN	7.847	7.841 ILE	41 HB	2.708	2.706 ASN	25 ND2	112.79	112.5
3326 GLY	43 HN	7.847	7.839 CYS	42 HB2	2.421	2.419 ASN	25 ND2	112.79	112.5
3327 GLY	10 HN	7.799	7.791 ASP	54 HB2	2.458	2.448 ASN	25 ND2	112.79	112.5
3328 GLY	10 HN	7.799	7.794 ASP	36 HB2	2.521	2.511 ASN	25 ND2	112.79	112.5
3329 GLY	10 HN	7.799	7.794 CYS	6 HA	2.753	2.757 ASN	25 ND2	112.79	112.5
3330 GLY	10 HN	7.799	7.791 CYS	42 HB2	2.421	2.413 ASN	25 ND2	112.79	112.5
3331 GLY	10 HN	7.799	7.792 ILE	41 HG11	1.414	1.404 ASN	25 ND2	112.79	112.5
3333 GLY	43 HN	7.847	7.839 VAL	38 HB	1.455	1.456 ASN	25 ND2	112.79	112.5
3334 GLY	43 HN	7.847	7.841 ALA	44 HB*	1.41	1.401 ASN	25 ND2	112.79	112.5
3336 GLY	10 HN	7.799	7.794 VAL	5 HG1*	0.775	0.765 ASN	25 ND2	112.79	112.5
3337 GLY	43 HN	7.847	7.841 VAL	5 HG1*	0.775	0.768 ASN	25 ND2	112.79	112.5
3338 GLY	43 HN	7.847	7.843 GLY	43 HN	7.847	7.845 ASN	25 ND2	112.79	112.5
3339 LYS	31 HN	8.673	8.662 TYR	13 HE1	6.416	6.413 ASN	14 ND2	112.58	112.25
3340 LYS	31 HN	8.673	8.661 THR	28 HA	4.072	4.066 ASN	14 ND2	112.58	112.25
3342 LYS	31 HN	8.673	8.663 PRO	45 HD2	3.509	3.519 ASN	14 ND2	112.58	112.25

3344 LYS	31 HN	8.673	8.661 GLY	27 HA2	3.374	3.372 ASN	14 ND2	112.58	112.25
3345 LYS	51 HN	7.909	7.904 SER	47 HA	4.363	4.358 SER	47 15N	109.53	109.5
3346 LYS	51 HN	7.909	7.904 PRO	45 HA	4.641	4.643 SER	47 15N	109.53	109.5
3347 LYS	51 HN	7.909	7.914 ASN	25 HA	4.698	4.696 SER	47 15N	109.53	109.5
3348 LYS	51 HN	7.909	7.904 LYS	46 HA	4.026	4.019 SER	47 15N	109.53	109.5
3349 LYS	51 HN	7.909	7.905 ASP	35 HA	4.135	4.129 SER	47 15N	109.53	109.5
3350 LYS	51 HN	7.909	7.905 PRO	15 HD1	3.915	3.906 SER	47 15N	109.53	109.5
3352 LYS	51 HN	7.909	7.903 PRO	45 HB1	2.351	2.34 SER	47 15N	109.53	109.5
3353 LYS	51 HN	7.909	7.904 PRO	26 HG2	1.97	1.964 SER	47 15N	109.53	109.5
3354 LYS	51 HN	7.909	7.904 PRO	45 HG1	2.021	2.026 SER	47 15N	109.53	109.5
3362 ASP	32 HN	7.544	7.528 PRO	20 HA	4.046	4.037 GLY	23 15N	104.53	104.5
3363 ASP	32 HN	7.544	7.529 VAL	24 HA	4.078	4.083 GLY	23 15N	104.53	104.5
3364 ASP	32 HN	7.544	7.528 GLY	23 HA2	3.75	3.747 GLY	23 15N	104.53	104.5

Ambiguous Assignment, multiple D2 assignments:

PeakNum Name	ResNum AtmNam Shift	D1Shift Name	ResNum AtmNam Shift	D2Shift Name	ResNum AtmNam Shift	D3Shift Distance
51 CYS	6 HN 9.201	9.196 TYR	11 HN 9.321	9.317 CYS	6 15N 131.19	131.171 3.7727
51 CYS	6 HN 9.201	9.196 GLU	50 HN 9.314	9.317 CYS	6 15N 131.19	131.171 5.1343
55 CYS	6 HN 9.201	9.198 CYS	6 HN 9.201	9.198 CYS	6 15N 131.19	131.173 0
55 CYS	6 HN 9.201	9.198 ASN	22 HD21 9.195	9.198 CYS	6 15N 131.19	131.173 13.142
61 LYS	7 HN 8.891	8.888 TYR	11 HN 9.321	9.311 LYS	7 15N 130.58	130.592 6.5111
61 LYS	7 HN 8.891	8.888 GLU	50 HN 9.314	9.311 LYS	7 15N 130.58	130.592 4.0808
72 ASP	29 HN 9.372	9.364 LYS	31 HN 8.673	8.668 ASP	29 15N 131.67	131.608 5.3657
72 ASP	29 HN 9.372	9.364 GLY	27 HN 8.667	8.668 ASP	29 15N 131.67	131.608 6.396
102 ASP	29 HN 9.372	9.367 ASP	32 HN 7.544	7.539 ASP	29 15N 131.67	131.645 4.2753
102 ASP	29 HN 9.372	9.367 PHE	49 HZ 7.54	7.539 ASP	29 15N 131.67	131.645 14.338
102 ASP	29 HN 9.372	9.367 GLY	23 HN 7.534	7.539 ASP	29 15N 131.67	131.645 13.432
103 CYS	6 HN 9.201	9.197 PHE	49 HE1 7.458	7.453 CYS	6 15N 131.19	131.205 6.1627
103 CYS	6 HN 9.201	9.197 PHE	49 HE2 7.458	7.453 CYS	6 15N 131.19	131.205 3.4028
105 CYS	6 HN 9.201	9.199 ASP	32 HN 7.544	7.536 CYS	6 15N 131.19	131.137 14.921
105 CYS	6 HN 9.201	9.199 PHE	49 HZ 7.54	7.536 CYS	6 15N 131.19	131.137 4.7687
105 CYS	6 HN 9.201	9.199 GLY	23 HN 7.534	7.536 CYS	6 15N 131.19	131.137 16.841
111 CYS	6 HN 9.201	9.198 TYR	11 HD1 7.312	7.305 CYS	6 15N 131.19	131.213 6.6409
111 CYS	6 HN 9.201	9.198 TYR	11 HD2 7.312	7.305 CYS	6 15N 131.19	131.213 3.7812
119 ASP	29 HN 9.372	9.369 THR	28 HN 6.972	6.966 ASP	29 15N 131.67	131.633 4.4853
119 ASP	29 HN 9.372	9.369 TYR	13 HD1 6.971	6.966 ASP	29 15N 131.67	131.633 9.852
119 ASP	29 HN 9.372	9.369 TYR	13 HD2 6.971	6.966 ASP	29 15N 131.67	131.633 7.8157

138 ASP	29 HN	9.372	9.368 ASP	29 HA	4.498	4.495 ASP	29 15N	131.67	131.654	2.8919
138 ASP	29 HN	9.372	9.368 ILE	12 HA	4.494	4.495 ASP	29 15N	131.67	131.654	14.48
139 CYS	6 HN	9.201	9.197 ASP	29 HA	4.498	4.488 CYS	6 15N	131.19	131.165	13.906
139 CYS	6 HN	9.201	9.197 ILE	12 HA	4.494	4.488 CYS	6 15N	131.19	131.165	3.2337
143 ASP	29 HN	9.372	9.369 THR	28 HA	4.072	4.065 ASP	29 15N	131.67	131.649	2.165
143 ASP	29 HN	9.372	9.369 TRP	37 HA	4.072	4.065 ASP	29 15N	131.67	131.649	13.986
143 ASP	29 HN	9.372	9.369 GLY	23 HA1	4.061	4.065 ASP	29 15N	131.67	131.649	12.872
150 ASP	29 HN	9.372	9.37 CYS	39 HA	3.695	3.688 ASP	29 15N	131.67	131.661	14.866
150 ASP	29 HN	9.372	9.37 THR	28 HB	3.688	3.688 ASP	29 15N	131.67	131.661	4.341
153 LYS	7 HN	8.891	8.888 LYS	7 HA	3.892	3.885 LYS	7 15N	130.58	130.555	2.8718
153 LYS	7 HN	8.891	8.888 PRO	15 HD2	3.883	3.885 LYS	7 15N	130.58	130.555	12.891
160 LYS	7 HN	8.891	8.89 ASN	22 HB1	2.93	2.94 LYS	7 15N	130.58	130.542	15.736
160 LYS	7 HN	8.891	8.89 ASN	22 HB2	2.93	2.94 LYS	7 15N	130.58	130.542	16.13
168 ASP	29 HN	9.372	9.369 ASP	32 HB2	2.364	2.36 ASP	29 15N	131.67	131.673	4.696
168 ASP	29 HN	9.372	9.369 ASN	25 HB2	2.359	2.36 ASP	29 15N	131.67	131.673	8.9292
168 ASP	29 HN	9.372	9.369 PRO	45 HB1	2.351	2.36 ASP	29 15N	131.67	131.673	17.386
168 ASP	29 HN	9.372	9.369 TRP	4 HB2	2.35	2.36 ASP	29 15N	131.67	131.673	11.759
172 CYS	6 HN	9.201	9.198 ASP	36 HB2	2.521	2.51 CYS	6 15N	131.19	131.167	18.062
172 CYS	6 HN	9.201	9.198 CYS	6 HB2	2.516	2.51 CYS	6 15N	131.19	131.167	2.8135
182 CYS	6 HN	9.201	9.197 VAL	5 HB	1.707	1.699 CYS	6 15N	131.19	131.165	4.1873
182 CYS	6 HN	9.201	9.197 LYS	3 HB1	1.706	1.699 CYS	6 15N	131.19	131.165	9.1471
183 LYS	7 HN	8.891	8.889 LYS	7 HB1	1.904	1.898 LYS	7 15N	130.58	130.575	2.4917
183 LYS	7 HN	8.891	8.889 LYS	7 HB2	1.904	1.898 LYS	7 15N	130.58	130.575	3.6243
184 LYS	7 HN	8.891	8.888 VAL	24 HB	1.799	1.791 LYS	7 15N	130.58	130.572	15.797
184 LYS	7 HN	8.891	8.888 LYS	7 HD1	1.798	1.791 LYS	7 15N	130.58	130.572	4.8671
184 LYS	7 HN	8.891	8.888 LYS	7 HD2	1.798	1.791 LYS	7 15N	130.58	130.572	4.8004
184 LYS	7 HN	8.891	8.888 PRO	15 HB1	1.794	1.791 LYS	7 15N	130.58	130.572	16.659
184 LYS	7 HN	8.891	8.888 LYS	2 HD1	1.789	1.791 LYS	7 15N	130.58	130.572	18.178
184 LYS	7 HN	8.891	8.888 LYS	2 HD2	1.789	1.791 LYS	7 15N	130.58	130.572	18.228
184 LYS	7 HN	8.891	8.888 PRO	40 HG1	1.787	1.791 LYS	7 15N	130.58	130.572	11.154
184 LYS	7 HN	8.891	8.888 ILE	12 HG11	1.784	1.791 LYS	7 15N	130.58	130.572	9.543
186 CYS	6 HN	9.201	9.201 ALA	44 HB*	1.41	1.402 CYS	6 15N	131.19	131.244	5.7207
186 CYS	6 HN	9.201	9.201 ILE	12 HB	1.399	1.402 CYS	6 15N	131.19	131.244	5.7751
187 LYS	7 HN	8.891	8.883 LYS	51 HD1	1.304	1.303 LYS	7 15N	130.58	130.626	12.273
187 LYS	7 HN	8.891	8.883 LYS	51 HD2	1.304	1.303 LYS	7 15N	130.58	130.626	13.022
188 LYS	7 HN	8.891	8.889 LYS	7 HG2	1.417	1.409 LYS	7 15N	130.58	130.556	2.382
188 LYS	7 HN	8.891	8.889 ILE	41 HG11	1.414	1.409 LYS	7 15N	130.58	130.556	10.239

188 LYS	7 HN	8.891	8.889 ILE	41 HG12	1.414	1.409 LYS	7 15N	130.58	130.556	10.53
188 LYS	7 HN	8.891	8.889 ALA	44 HB*	1.41	1.409 LYS	7 15N	130.58	130.556	10.53
188 LYS	7 HN	8.891	8.889 ILE	12 HB	1.399	1.409 LYS	7 15N	130.58	130.556	10.034
189 TRP	4 HE1	9.818	9.814 LYS	51 HD1	1.304	1.294 TRP	4 NE1	129.31	129.324	4.3191
189 TRP	4 HE1	9.818	9.814 LYS	51 HD2	1.304	1.294 TRP	4 NE1	129.31	129.324	5.5595
189 TRP	4 HE1	9.818	9.814 ILE	8 HG11	1.288	1.294 TRP	4 NE1	129.31	129.324	15.402
189 TRP	4 HE1	9.818	9.814 ILE	8 HG12	1.288	1.294 TRP	4 NE1	129.31	129.324	16.839
194 CYS	6 HN	9.201	9.197 VAL	5 HG1*	0.775	0.766 CYS	6 15N	131.19	131.164	8.5428
194 CYS	6 HN	9.201	9.197 VAL	5 HG2*	0.775	0.766 CYS	6 15N	131.19	131.164	8.5428
194 CYS	6 HN	9.201	9.197 ILE	41 HD1*	0.773	0.766 CYS	6 15N	131.19	131.164	8.5428
194 CYS	6 HN	9.201	9.197 LYS	51 HB1	0.761	0.766 CYS	6 15N	131.19	131.164	10.271
194 CYS	6 HN	9.201	9.197 LYS	51 HB2	0.761	0.766 CYS	6 15N	131.19	131.164	10.949
194 CYS	6 HN	9.201	9.197 ILE	8 HG2*	0.755	0.766 CYS	6 15N	131.19	131.164	10.949
196 LYS	7 HN	8.891	8.889 VAL	5 HG1*	0.775	0.767 LYS	7 15N	130.58	130.503	10.711
196 LYS	7 HN	8.891	8.889 VAL	5 HG2*	0.775	0.767 LYS	7 15N	130.58	130.503	10.711
196 LYS	7 HN	8.891	8.889 ILE	41 HD1*	0.773	0.767 LYS	7 15N	130.58	130.503	10.711
196 LYS	7 HN	8.891	8.889 LYS	51 HB1	0.761	0.767 LYS	7 15N	130.58	130.503	10.08
196 LYS	7 HN	8.891	8.889 LYS	51 HB2	0.761	0.767 LYS	7 15N	130.58	130.503	10.711
255 TRP	4 HE1	9.818	9.814 PHE	30 HN	9.033	9.028 TRP	4 NE1	129.31	129.223	3.2245
255 TRP	4 HE1	9.818	9.814 ALA	44 HN	9.031	9.028 TRP	4 NE1	129.31	129.223	16.189
328 TRP	4 HE1	9.818	9.812 LYS	31 HN	8.673	8.671 TRP	4 NE1	129.31	129.183	4.9412
328 TRP	4 HE1	9.818	9.812 GLY	27 HN	8.667	8.671 TRP	4 NE1	129.31	129.183	10.133
439 LEU	52 HN	8.324	8.324 LYS	51 HN	7.909	7.904 LEU	52 15N	126.74	126.631	4.6187
439 LEU	52 HN	8.324	8.324 SER	47 HN	7.908	7.904 LEU	52 15N	126.74	126.631	14.013
503 TRP	4 HE1	9.818	9.814 TRP	4 HZ2	7.372	7.368 TRP	4 NE1	129.31	129.262	2.9107
503 TRP	4 HE1	9.818	9.814 VAL	24 HN	7.365	7.368 TRP	4 NE1	129.31	129.262	14.288
552 ASN	25 HN	8.766	8.764 THR	28 HN	6.972	6.97 ASN	25 15N	127.19	127.202	5.2894
552 ASN	25 HN	8.766	8.764 TYR	13 HD1	6.971	6.97 ASN	25 15N	127.19	127.202	9.1103
552 ASN	25 HN	8.766	8.764 TYR	13 HD2	6.971	6.97 ASN	25 15N	127.19	127.202	10.743
553 ASN	25 HN	8.766	8.762 TRP	4 HZ3	6.924	6.914 ASN	25 15N	127.19	127.171	16.952
553 ASN	25 HN	8.766	8.762 ASN	25 HD22	6.916	6.914 ASN	25 15N	127.19	127.171	4.512
563 ASN	25 HN	8.766	8.763 TYR	13 HE1	6.416	6.408 ASN	25 15N	127.19	127.15	6.7423
563 ASN	25 HN	8.766	8.763 TYR	13 HE2	6.416	6.408 ASN	25 15N	127.19	127.15	8.8073
575 LEU	52 HN	8.324	8.321 TRP	4 HA	5.05	5.044 LEU	52 15N	126.74	126.741	2.546
575 LEU	52 HN	8.324	8.321 ASN	14 HA	5.045	5.044 LEU	52 15N	126.74	126.741	7.703
606 ASN	25 HN	8.766	8.763 VAL	24 HA	4.078	4.072 ASN	25 15N	127.19	127.156	2.1767
606 ASN	25 HN	8.766	8.763 THR	28 HA	4.072	4.072 ASN	25 15N	127.19	127.156	6.1394

606 ASN	25 HN	8.766	8.763 TRP	37 HA	4.072	4.072 ASN	25 15N	127.19	127.156	10.875
606 ASN	25 HN	8.766	8.763 GLY	23 HA1	4.061	4.072 ASN	25 15N	127.19	127.156	5.0457
645 TRP	4 HE1	9.818	9.813 ASP	36 HB1	2.733	2.724 TRP	4 NE1	129.31	129.254	18.211
645 TRP	4 HE1	9.818	9.813 LYS	51 HE1	2.728	2.724 TRP	4 NE1	129.31	129.254	4.6022
645 TRP	4 HE1	9.818	9.813 LYS	51 HE2	2.728	2.724 TRP	4 NE1	129.31	129.254	2.976
645 TRP	4 HE1	9.818	9.813 ASP	17 HB1	2.725	2.724 TRP	4 NE1	129.31	129.254	11.21
646 TRP	4 HE1	9.818	9.813 CYS	42 HB2	2.421	2.411 TRP	4 NE1	129.31	129.248	17.868
646 TRP	4 HE1	9.818	9.813 GLU	48 HG2	2.405	2.411 TRP	4 NE1	129.31	129.248	15.765
650 PHE	30 HN	9.033	9.026 ASP	36 HB2	2.521	2.518 PHE	30 15N	127.95	127.902	16.097
650 PHE	30 HN	9.033	9.026 CYS	6 HB2	2.516	2.518 PHE	30 15N	127.95	127.902	14.126
653 PHE	30 HN	9.033	9.022 ASP	29 HB1	2.633	2.627 PHE	30 15N	127.95	127.768	4.2906
653 PHE	30 HN	9.033	9.022 TRP	4 HB1	2.617	2.627 PHE	30 15N	127.95	127.768	6.5039
653 PHE	30 HN	9.033	9.022 ASP	17 HB2	2.617	2.627 PHE	30 15N	127.95	127.768	12.336
653 PHE	30 HN	9.033	9.022 ASP	35 HB1	2.617	2.627 PHE	30 15N	127.95	127.768	13.005
664 ASN	25 HN	8.766	8.763 ASN	25 HB2	2.359	2.352 ASN	25 15N	127.19	127.163	3.613
664 ASN	25 HN	8.766	8.763 PRO	45 HB1	2.351	2.352 ASN	25 15N	127.19	127.163	17.892
664 ASN	25 HN	8.766	8.763 TRP	4 HB2	2.35	2.352 ASN	25 15N	127.19	127.163	15.218
671 ASN	25 HN	8.766	8.764 VAL	24 HB	1.799	1.798 ASN	25 15N	127.19	127.121	4.4254
671 ASN	25 HN	8.766	8.764 LYS	7 HD1	1.798	1.798 ASN	25 15N	127.19	127.121	23.766
671 ASN	25 HN	8.766	8.764 LYS	7 HD2	1.798	1.798 ASN	25 15N	127.19	127.121	22.653
671 ASN	25 HN	8.766	8.764 PRO	15 HB1	1.794	1.798 ASN	25 15N	127.19	127.121	9.7534
671 ASN	25 HN	8.766	8.764 LYS	2 HD1	1.789	1.798 ASN	25 15N	127.19	127.121	15.071
671 ASN	25 HN	8.766	8.764 LYS	2 HD2	1.789	1.798 ASN	25 15N	127.19	127.121	16.702
671 ASN	25 HN	8.766	8.764 PRO	40 HG1	1.787	1.798 ASN	25 15N	127.19	127.121	12.964
673 LEU	52 HN	8.324	8.325 PRO	34 HB2	1.85	1.845 LEU	52 15N	126.74	126.745	19.849
673 LEU	52 HN	8.324	8.325 PRO	34 HG2	1.85	1.845 LEU	52 15N	126.74	126.745	19.297
673 LEU	52 HN	8.324	8.325 GLU	50 HB1	1.835	1.845 LEU	52 15N	126.74	126.745	7.2875
673 LEU	52 HN	8.324	8.325 GLU	50 HB2	1.835	1.845 LEU	52 15N	126.74	126.745	6.1232
675 LEU	52 HN	8.324	8.323 LYS	31 HB1	1.712	1.703 LEU	52 15N	126.74	126.706	12.559
675 LEU	52 HN	8.324	8.323 LYS	31 HB2	1.712	1.703 LEU	52 15N	126.74	126.706	11.022
675 LEU	52 HN	8.324	8.323 PRO	26 HB2	1.711	1.703 LEU	52 15N	126.74	126.706	16.434
675 LEU	52 HN	8.324	8.323 VAL	5 HB	1.707	1.703 LEU	52 15N	126.74	126.706	5.7896
675 LEU	52 HN	8.324	8.323 LYS	3 HB1	1.706	1.703 LEU	52 15N	126.74	126.706	4.2687
680 ASP	54 HN	7.829	7.826 GLU	53 HB2	1.723	1.715 ASP	54 15N	125.73	125.752	3.9458
680 ASP	54 HN	7.829	7.826 LYS	31 HB1	1.712	1.715 ASP	54 15N	125.73	125.752	16.943
680 ASP	54 HN	7.829	7.826 LYS	31 HB2	1.712	1.715 ASP	54 15N	125.73	125.752	15.409
680 ASP	54 HN	7.829	7.826 PRO	26 HB2	1.711	1.715 ASP	54 15N	125.73	125.752	21.974

680 ASP	54 HN	7.829	7.826 VAL	5 HB	1.707	1.715 ASP	54 15N	125.73	125.752	11.766
680 ASP	54 HN	7.829	7.826 LYS	3 HB1	1.706	1.715 ASP	54 15N	125.73	125.752	9.595
682 TRP	4 HE1	9.818	9.813 LYS	7 HG2	1.417	1.414 TRP	4 NE1	129.31	129.214	11.631
682 TRP	4 HE1	9.818	9.813 ILE	41 HG11	1.414	1.414 TRP	4 NE1	129.31	129.214	15.218
682 TRP	4 HE1	9.818	9.813 ILE	41 HG12	1.414	1.414 TRP	4 NE1	129.31	129.214	16.09
682 TRP	4 HE1	9.818	9.813 ALA	44 HB*	1.41	1.414 TRP	4 NE1	129.31	129.214	16.09
693 LEU	52 HN	8.324	8.321 LEU	52 HB2	1.216	1.211 LEU	52 15N	126.74	126.741	3.6295
693 LEU	52 HN	8.324	8.321 LYS	31 HG1	1.202	1.211 LEU	52 15N	126.74	126.741	12.511
693 LEU	52 HN	8.324	8.321 LYS	31 HG2	1.202	1.211 LEU	52 15N	126.74	126.741	13.811
698 ASP	54 HN	7.829	7.825 LYS	31 HD1	1.566	1.567 ASP	54 15N	125.73	125.727	16.565
698 ASP	54 HN	7.829	7.825 LYS	3 HD2	1.563	1.567 ASP	54 15N	125.73	125.727	10.111
708 ASN	25 HN	8.766	8.762 VAL	38 HG1*	0.508	0.497 ASN	25 15N	127.19	127.161	17.157
708 ASN	25 HN	8.766	8.762 VAL	24 HG2*	0.503	0.497 ASN	25 15N	127.19	127.161	17.157
808 ILE	41 HN	8.685	8.678 ILE	41 HN	8.685	8.68 ILE	41 15N	121.87	121.881	0
808 ILE	41 HN	8.685	8.678 LYS	31 HN	8.673	8.68 ILE	41 15N	121.87	121.881	16.579
905 TRP	37 HN	7.558	7.554 TRP	37 HN	7.558	7.554 TRP	37 15N	124.38	124.383	0
905 TRP	37 HN	7.558	7.554 ASP	32 HN	7.544	7.554 TRP	37 15N	124.38	124.383	9.974
958 TRP	37 HN	7.558	7.553 ASN	22 HD22	6.987	6.983 TRP	37 15N	124.38	124.399	9.9577
958 TRP	37 HN	7.558	7.553 TRP	37 HD1	6.984	6.983 TRP	37 15N	124.38	124.399	5.1303
958 TRP	37 HN	7.558	7.553 THR	28 HN	6.972	6.983 TRP	37 15N	124.38	124.399	13.343
958 TRP	37 HN	7.558	7.553 TYR	13 HD1	6.971	6.983 TRP	37 15N	124.38	124.399	10.45
958 TRP	37 HN	7.558	7.553 TYR	13 HD2	6.971	6.983 TRP	37 15N	124.38	124.399	11.929
994 TRP	37 HN	7.558	7.554 TRP	37 HE3	6.542	6.535 TRP	37 15N	124.38	124.394	4.5918
994 TRP	37 HN	7.558	7.554 TRP	4 HE3	6.529	6.535 TRP	37 15N	124.38	124.394	12.765
1014 TRP	37 HN	7.558	7.554 ASP	36 HA	4.459	4.454 TRP	37 15N	124.38	124.38	3.3009
1014 TRP	37 HN	7.558	7.554 LYS	2 HA	4.457	4.454 TRP	37 15N	124.38	124.38	18.873
1026 GLU	53 HN	8.217	8.213 LEU	52 HA	4.208	4.199 GLU	53 15N	122.56	122.568	2.3326
1026 GLU	53 HN	8.217	8.213 GLU	53 HA	4.19	4.199 GLU	53 15N	122.56	122.568	2.8755
1042 ILE	41 HN	8.685	8.676 CYS	39 HA	3.695	3.69 ILE	41 15N	121.87	121.884	3.78
1042 ILE	41 HN	8.685	8.676 THR	28 HB	3.684	3.69 ILE	41 15N	121.87	121.884	14.635
1046 TRP	37 HN	7.558	7.555 CYS	9 HB1	3.199	3.192 TRP	37 15N	124.38	124.375	16.644
1046 TRP	37 HN	7.558	7.555 PRO	34 HD2	3.189	3.192 TRP	37 15N	124.38	124.375	6.2682
1058 ILE	41 HN	8.685	8.676 CYS	39 HB2	2.968	2.958 ILE	41 15N	121.87	121.868	4.1478
1058 ILE	41 HN	8.685	8.676 CYS	6 HB1	2.954	2.958 ILE	41 15N	121.87	121.868	5.3498
1074 TRP	37 HN	7.558	7.554 PRO	34 HB1	2.295	2.291 TRP	37 15N	124.38	124.407	3.3606
1074 TRP	37 HN	7.558	7.554 PRO	45 HB2	2.283	2.291 TRP	37 15N	124.38	124.407	7.3925
1074 TRP	37 HN	7.558	7.554 PRO	20 HB1	2.282	2.291 TRP	37 15N	124.38	124.407	15.029

1077 GLU	53 HN	8.217	8.214 GLU	53 HG1	2.161	2.15 GLU	53 15N	122.56	122.533	2.6362
1077 GLU	53 HN	8.217	8.214 GLU	16 HG2	2.158	2.15 GLU	53 15N	122.56	122.533	15.283
1078 GLU	53 HN	8.217	8.214 GLU	53 HG2	2.071	2.066 GLU	53 15N	122.56	122.553	3.4475
1078 GLU	53 HN	8.217	8.214 PRO	26 HG1	2.058	2.066 GLU	53 15N	122.56	122.553	22.367
1084 TRP	37 HN	7.558	7.554 PRO	26 HG2	1.97	1.959 TRP	37 15N	124.38	124.357	16.482
1084 TRP	37 HN	7.558	7.554 GLU	53 HB1	1.96	1.959 TRP	37 15N	124.38	124.357	22.523
1085 TRP	37 HN	7.558	7.555 LYS	46 HB1	1.862	1.853 TRP	37 15N	124.38	124.321	6.1518
1085 TRP	37 HN	7.558	7.555 LYS	46 HB2	1.862	1.853 TRP	37 15N	124.38	124.321	6.9381
1085 TRP	37 HN	7.558	7.555 PRO	34 HB2	1.85	1.853 TRP	37 15N	124.38	124.321	4.6687
1085 TRP	37 HN	7.558	7.555 PRO	34 HG2	1.85	1.853 TRP	37 15N	124.38	124.321	6.2079
1090 GLU	53 HN	8.217	8.214 GLU	53 HB2	1.723	1.713 GLU	53 15N	122.56	122.576	3.4328
1090 GLU	53 HN	8.217	8.214 LYS	31 HB1	1.712	1.713 GLU	53 15N	122.56	122.576	14.379
1090 GLU	53 HN	8.217	8.214 LYS	31 HB2	1.712	1.713 GLU	53 15N	122.56	122.576	12.893
1090 GLU	53 HN	8.217	8.214 PRO	26 HB2	1.711	1.713 GLU	53 15N	122.56	122.576	19.886
1090 GLU	53 HN	8.217	8.214 VAL	5 HB	1.707	1.713 GLU	53 15N	122.56	122.576	7.9972
1090 GLU	53 HN	8.217	8.214 LYS	3 HB1	1.706	1.713 GLU	53 15N	122.56	122.576	7.1308
1093 ILE	41 HN	8.685	8.685 LYS	2 HD1	1.789	1.78 ILE	41 15N	121.87	121.865	21.128
1093 ILE	41 HN	8.685	8.685 LYS	2 HD2	1.789	1.78 ILE	41 15N	121.87	121.865	21.842
1093 ILE	41 HN	8.685	8.685 PRO	40 HG1	1.787	1.78 ILE	41 15N	121.87	121.865	3.0189
1093 ILE	41 HN	8.685	8.685 ILE	12 HG11	1.784	1.78 ILE	41 15N	121.87	121.865	11.469
1094 ILE	41 HN	8.685	8.681 PRO	40 HB2	1.642	1.636 ILE	41 15N	121.87	121.89	4.421
1094 ILE	41 HN	8.685	8.681 LYS	3 HD1	1.633	1.636 ILE	41 15N	121.87	121.89	16.959
1106 ILE	41 HN	8.685	8.678 LYS	7 HG2	1.417	1.406 ILE	41 15N	121.87	121.866	12.181
1106 ILE	41 HN	8.685	8.678 ILE	41 HG11	1.414	1.406 ILE	41 15N	121.87	121.866	2.4625
1106 ILE	41 HN	8.685	8.678 ILE	41 HG12	1.414	1.406 ILE	41 15N	121.87	121.866	3.9133
1106 ILE	41 HN	8.685	8.678 ALA	44 HB*	1.41	1.406 ILE	41 15N	121.87	121.866	3.9133
1106 ILE	41 HN	8.685	8.678 ILE	12 HB	1.399	1.406 ILE	41 15N	121.87	121.866	10.281
1108 ILE	41 HN	8.685	8.678 LYS	31 HG1	1.202	1.195 ILE	41 15N	121.87	121.879	19.024
1108 ILE	41 HN	8.685	8.678 LYS	31 HG2	1.202	1.195 ILE	41 15N	121.87	121.879	19.472
1126 TRP	37 HN	7.558	7.555 VAL	38 HG1*	0.508	0.502 TRP	37 15N	124.38	124.404	11.805
1126 TRP	37 HN	7.558	7.555 VAL	24 HG2*	0.503	0.502 TRP	37 15N	124.38	124.404	11.805
1129 ILE	41 HN	8.685	8.676 VAL	5 HG1*	0.775	0.767 ILE	41 15N	121.87	121.865	19.472
1129 ILE	41 HN	8.685	8.676 VAL	5 HG2*	0.775	0.767 ILE	41 15N	121.87	121.865	19.472
1129 ILE	41 HN	8.685	8.676 ILE	41 HD1*	0.773	0.767 ILE	41 15N	121.87	121.865	19.472
1129 ILE	41 HN	8.685	8.676 LYS	51 HB1	0.761	0.767 ILE	41 15N	121.87	121.865	16.661
1129 ILE	41 HN	8.685	8.676 LYS	51 HB2	0.761	0.767 ILE	41 15N	121.87	121.865	17.827
1131 ILE	41 HN	8.685	8.674 ILE	41 HG2*	0.684	0.68 ILE	41 15N	121.87	121.865	17.827

1131 ILE	41 HN	8.685	8.674 VAL	24 HG1*	0.672	0.68 ILE	41 15N	121.87	121.865	17.827
1469 PHE	49 HN	7.744	7.74 LYS	51 HN	7.909	7.904 PHE	49 15N	118.65	118.692	7.0925
1469 PHE	49 HN	7.744	7.74 SER	47 HN	7.908	7.904 PHE	49 15N	118.65	118.692	4.4139
1474 LYS	46 HN	8.532	8.528 LYS	51 HN	7.909	7.904 LYS	46 15N	118.16	118.167	12.248
1474 LYS	46 HN	8.532	8.528 SER	47 HN	7.908	7.904 LYS	46 15N	118.16	118.167	2.9204
1530 PHE	49 HN	7.744	7.737 PHE	49 HE1	7.458	7.452 PHE	49 15N	118.65	118.613	5.0472
1530 PHE	49 HN	7.744	7.737 PHE	49 HE2	7.458	7.452 PHE	49 15N	118.65	118.613	6.7506
1548 ASP	35 HN	8.247	8.246 TRP	37 HN	7.558	7.553 ASP	35 15N	117.66	117.659	4.3063
1548 ASP	35 HN	8.247	8.246 ASP	32 HN	7.544	7.553 ASP	35 15N	117.66	117.659	8.5895
1585 PHE	49 HN	7.744	7.739 PHE	49 HD1	7.258	7.267 PHE	49 15N	118.65	118.633	2.6579
1585 PHE	49 HN	7.744	7.739 PHE	49 HD2	7.258	7.267 PHE	49 15N	118.65	118.633	5.2203
1643 LYS	46 HN	8.532	8.528 TRP	37 HE3	6.542	6.537 LYS	46 15N	118.16	118.164	4.4547
1643 LYS	46 HN	8.532	8.528 TRP	4 HE3	6.529	6.537 LYS	46 15N	118.16	118.164	9.4741
1646 PHE	49 HN	7.744	7.743 PHE	30 HE1	6.059	6.054 PHE	49 15N	118.65	118.609	4.6209
1646 PHE	49 HN	7.744	7.743 PHE	30 HE2	6.059	6.054 PHE	49 15N	118.65	118.609	6.1217
1673 LYS	3 HN	8.607	8.595 TRP	4 HA	5.05	5.041 LYS	3 15N	120.48	120.251	4.9549
1673 LYS	3 HN	8.607	8.595 ASN	14 HA	5.045	5.041 LYS	3 15N	120.48	120.251	5.2897
1679 TRP	4 HN	8.376	8.371 TRP	4 HA	5.05	5.044 TRP	4 15N	119.19	119.206	2.988
1679 TRP	4 HN	8.376	8.371 ASN	14 HA	5.045	5.044 TRP	4 15N	119.19	119.206	4.0484
1692 ASP	21 HN	9.336	9.334 TYR	13 HA	4.396	4.393 ASP	21 15N	120.1	120.097	10.452
1692 ASP	21 HN	9.336	9.334 ASP	21 HA	4.394	4.393 ASP	21 15N	120.1	120.097	2.9008
1701 PHE	49 HN	7.744	7.738 SER	47 HA	4.363	4.357 PHE	49 15N	118.65	118.655	3.7119
1701 PHE	49 HN	7.744	7.738 VAL	38 HA	4.356	4.357 PHE	49 15N	118.65	118.655	7.9571
1705 LYS	46 HN	8.532	8.527 SER	47 HA	4.363	4.352 LYS	46 15N	118.16	118.162	5.4497
1705 LYS	46 HN	8.532	8.527 VAL	38 HA	4.356	4.352 LYS	46 15N	118.16	118.162	3.9671
1707 ASP	35 HN	8.247	8.243 ASP	36 HA	4.459	4.454 ASP	35 15N	117.66	117.66	5.4035
1707 ASP	35 HN	8.247	8.243 LYS	2 HA	4.457	4.454 ASP	35 15N	117.66	117.66	19.307
1723 LYS	46 HN	8.532	8.52 ASP	35 HA	4.135	4.129 LYS	46 15N	118.16	118.109	5.1982
1723 LYS	46 HN	8.532	8.52 SER	47 HB1	4.134	4.129 LYS	46 15N	118.16	118.109	6.4724
1739 ASP	21 HN	9.336	9.334 PRO	15 HD1	3.915	3.907 ASP	21 15N	120.1	120.096	14.113
1739 ASP	21 HN	9.336	9.334 PRO	20 HD1	3.911	3.907 ASP	21 15N	120.1	120.096	3.2296
1739 ASP	21 HN	9.336	9.334 SER	47 HB2	3.911	3.907 ASP	21 15N	120.1	120.096	21.414
1744 TRP	4 HN	8.376	8.373 PRO	15 HD1	3.915	3.914 TRP	4 15N	119.19	119.182	4.9843
1744 TRP	4 HN	8.376	8.373 PRO	20 HD1	3.911	3.914 TRP	4 15N	119.19	119.182	12.676
1744 TRP	4 HN	8.376	8.373 SER	47 HB2	3.911	3.914 TRP	4 15N	119.19	119.182	14.861
1745 PHE	49 HN	7.744	7.737 PRO	15 HD1	3.915	3.909 PHE	49 15N	118.65	118.615	13.886
1745 PHE	49 HN	7.744	7.737 PRO	20 HD1	3.911	3.909 PHE	49 15N	118.65	118.615	17.729

1745 PHE	49 HN	7.744	7.737 SER	47 HB2	3.911	3.909 PHE	49 15N	118.65	118.615	5.6207
1749 ASP	35 HN	8.247	8.248 PRO	34 HD1	3.659	3.654 ASP	35 15N	117.66	117.732	5.4864
1749 ASP	35 HN	8.247	8.248 PHE	49 HB1	3.645	3.654 ASP	35 15N	117.66	117.732	11.823
1777 ASP	21 HN	9.336	9..31 ASN	22 HB1	2.93	2.924 ASP	21 15N	120.1	120.081	4.8719
1777 ASP	21 HN	9.336	9.331 ASN	22 HB2	2.93	2.924 ASP	21 15N	120.1	120.081	6.2379
1799 TRP	4 HN	8.376	8.372 TRP	4 HB1	2.617	2.606 TRP	4 15N	119.19	119.196	2.6298
1799 TRP	4 HN	8.376	8.372 ASP	17 HB2	2.617	2.606 TRP	4 15N	119.19	119.196	10.422
1799 TRP	4 HN	8.376	8.372 ASP	35 HB1	2.617	2.606 TRP	4 15N	119.19	119.196	17.268
1799 TRP	4 HN	8.376	8.372 PHE	49 HB2	2.608	2.606 TRP	4 15N	119.19	119.196	6.1474
1815 TRP	4 HN	8.376	8.373 PRO	45 HB1	2.351	2.341 TRP	4 15N	119.19	119.196	14.837
1815 TRP	4 HN	8.376	8.373 TRP	4 HB2	2.35	2.341 TRP	4 15N	119.19	119.196	3.7578
1821 ASP	35 HN	8.247	8.244 PRO	34 HB1	2.295	2.289 ASP	35 15N	117.66	117.671	3.8684
1821 ASP	35 HN	8.247	8.244 PRO	45 HB2	2.283	2.289 ASP	35 15N	117.66	117.671	9.8236
1821 ASP	35 HN	8.247	8.244 PRO	20 HB1	2.282	2.289 ASP	35 15N	117.66	117.671	17.262
1840 ASP	35 HN	8.247	8.244 PRO	34 HB2	1.85	1.849 ASP	35 15N	117.66	117.71	3.3567
1840 ASP	35 HN	8.247	8.244 PRO	34 HG2	1.85	1.849 ASP	35 15N	117.66	117.71	4.9137
1852 PHE	49 HN	7.744	7.744 ILE	41 HG11	1.414	1.403 PHE	49 15N	118.65	118.616	12.333
1852 PHE	49 HN	7.744	7.744 ILE	41 HG12	1.414	1.403 PHE	49 15N	118.65	118.616	13.22
1852 PHE	49 HN	7.744	7.744 ALA	44 HB*	1.41	1.403 PHE	49 15N	118.65	118.616	13.22
1852 PHE	49 HN	7.744	7.744 ILE	12 HB	1.399	1.403 PHE	49 15N	118.65	118.616	12.501
1881 LYS	46 HN	8.532	8.528 VAL	38 HG1*	0.508	0.503 LYS	46 15N	118.16	118.148	15.506
1881 LYS	46 HN	8.532	8.528 VAL	24 HG2*	0.503	0.503 LYS	46 15N	118.16	118.148	15.506
2043 ASP	32 HN	7.544	7.539 ASP	32 HN	7.544	7.539 ASP	32 15N	116.48	116.479	0
2043 ASP	32 HN	7.544	7.539 PHE	49 HZ	7.54	7.539 ASP	32 15N	116.48	116.479	12.656
2043 ASP	32 HN	7.544	7.539 GLY	23 HN	7.534	7.539 ASP	32 15N	116.48	116.479	13.892
2057 VAL	38 HN	6.294	6.29 TRP	37 HN	7.558	7.554 VAL	38 15N	116.07	116.018	4.5663
2057 VAL	38 HN	6.294	6.29 ASP	32 HN	7.544	7.554 VAL	38 15N	116.07	116.018	12.24
2077 ASP	36 HN	8.089	8.085 TRP	37 HN	7.558	7.554 ASP	36 15N	114.21	114.224	2.2622
2077 ASP	36 HN	8.089	8.085 ASP	32 HN	7.544	7.554 ASP	36 15N	114.21	114.224	10.478
2191 VAL	38 HN	6.294	6.294 TRP	37 HE3	6.542	6.535 VAL	38 15N	116.07	116.033	3.8125
2191 VAL	38 HN	6.294	6.294 TRP	4 HE3	6.529	6.535 VAL	38 15N	116.07	116.033	12.614
2221 GLU	16 HN	7.488	7.481 TRP	4 HA	5.05	5.038 GLU	16 15N	113.61	113.316	10.25
2221 GLU	16 HN	7.488	7.481 ASN	14 HA	5.045	5.038 GLU	16 15N	113.61	113.316	3.7572
2224 VAL	38 HN	6.294	6.287 SER	47 HA	4.363	4.353 VAL	38 15N	116.07	116.08	11.453
2224 VAL	38 HN	6.294	6.287 VAL	38 HA	4.356	4.353 VAL	38 15N	116.07	116.08	2.9606
2231 ASP	36 HN	8.089	8.082 ASP	36 HA	4.459	4.455 ASP	36 15N	114.21	114.208	2.9611
2231 ASP	36 HN	8.089	8.082 LYS	2 HA	4.457	4.455 ASP	36 15N	114.21	114.208	20.328

2240 VAL	38 HN	6.294	6.29 VAL	24 HA	4.078	4.069 VAL	38 15N	116.07	116.077	9.3741
2240 VAL	38 HN	6.294	6.29 THR	28 HA	4.072	4.069 VAL	38 15N	116.07	116.077	13.98
2240 VAL	38 HN	6.294	6.29 TRP	37 HA	4.072	4.069 VAL	38 15N	116.07	116.077	2.2741
2240 VAL	38 HN	6.294	6.29 GLY	23 HA1	4.061	4.069 VAL	38 15N	116.07	116.077	10.427
2271 VAL	38 HN	6.294	6.293 ASN	22 HB1	2.93	2.936 VAL	38 15N	116.07	116.097	5.9156
2271 VAL	38 HN	6.294	6.293 ASN	22 HB2	2.93	2.936 VAL	38 15N	116.07	116.097	5.1925
2272 VAL	38 HN	6.294	6.29 ASP	19 HB2	2.819	2.816 VAL	38 15N	116.07	116.066	7.0359
2272 VAL	38 HN	6.294	6.29 TRP	37 HB1	2.814	2.816 VAL	38 15N	116.07	116.066	3.8333
2272 VAL	38 HN	6.294	6.29 TRP	37 HB2	2.814	2.816 VAL	38 15N	116.07	116.066	3.6764
2279 ASP	32 HN	7.544	7.539 ASP	29 HB2	2.531	2.524 ASP	32 15N	116.48	116.491	2.9387
2279 ASP	32 HN	7.544	7.539 ASP	36 HB2	2.521	2.524 ASP	32 15N	116.48	116.491	13.399
2279 ASP	32 HN	7.544	7.539 CYS	6 HB2	2.516	2.524 ASP	32 15N	116.48	116.491	16.356
2300 ASP	36 HN	8.089	8.085 PRO	34 HB1	2.295	2.29 ASP	36 15N	114.21	114.203	3.1547
2300 ASP	36 HN	8.089	8.085 PRO	45 HB2	2.283	2.29 ASP	36 15N	114.21	114.203	8.2175
2300 ASP	36 HN	8.089	8.085 PRO	20 HB1	2.282	2.29 ASP	36 15N	114.21	114.203	16.422
2317 ASP	36 HN	8.089	8.085 PRO	34 HB2	1.85	1.848 ASP	36 15N	114.21	114.197	3.5833
2317 ASP	36 HN	8.089	8.085 PRO	34 HG2	1.85	1.848 ASP	36 15N	114.21	114.197	5.7181
2320 GLU	16 HN	7.488	7.484 GLU	50 HB1	1.835	1.832 GLU	16 15N	113.61	113.609	16.637
2320 GLU	16 HN	7.488	7.484 GLU	50 HB2	1.835	1.832 GLU	16 15N	113.61	113.609	15.447
2320 GLU	16 HN	7.488	7.484 GLU	16 HB1	1.832	1.832 GLU	16 15N	113.61	113.609	2.1896
2321 GLU	16 HN	7.488	7.483 GLU	16 HB2	1.741	1.733 GLU	16 15N	113.61	113.59	3.4079
2321 GLU	16 HN	7.488	7.483 GLU	53 HB2	1.723	1.733 GLU	16 15N	113.61	113.59	12.389
2323 ASP	32 HN	7.544	7.536 LYS	31 HD1	1.566	1.564 ASP	32 15N	116.48	116.469	5.6476
2323 ASP	32 HN	7.544	7.536 LYS	3 HD2	1.563	1.564 ASP	32 15N	116.48	116.469	14.696
2335 VAL	38 HN	6.294	6.289 VAL	38 HG1*	0.508	0.503 VAL	38 15N	116.07	116.059	18.88
2335 VAL	38 HN	6.294	6.289 VAL	24 HG2*	0.503	0.503 VAL	38 15N	116.07	116.059	18.88
2338 ASP	36 HN	8.089	8.074 VAL	38 HG1*	0.508	0.504 ASP	36 15N	114.21	114.306	21.988
2338 ASP	36 HN	8.089	8.074 VAL	24 HG2*	0.503	0.504 ASP	36 15N	114.21	114.306	21.988
2749 ASN	25 HD21	7.586	7.578 VAL	24 HA	4.078	4.069 ASN	25 ND2	112.79	112.772	6.4843
2749 ASN	25 HD21	7.586	7.578 THR	28 HA	4.072	4.069 ASN	25 ND2	112.79	112.772	9.239
2749 ASN	25 HD21	7.586	7.578 TRP	37 HA	4.072	4.069 ASN	25 ND2	112.79	112.772	14.541
2749 ASN	25 HD21	7.586	7.578 GLY	23 HA1	4.061	4.069 ASN	25 ND2	112.79	112.772	6.0458
2803 ASN	25 HD21	7.586	7.582 ASN	25 HB2	2.359	2.352 ASN	25 ND2	112.79	112.775	3.6173
2803 ASN	25 HD21	7.586	7.582 PRO	45 HB1	2.351	2.352 ASN	25 ND2	112.79	112.775	22.161
2803 ASN	25 HD21	7.586	7.582 TRP	4 HB2	2.35	2.352 ASN	25 ND2	112.79	112.775	19.806
2913 GLY	18 HN	7.944	7.94 GLU	50 HB1	1.835	1.836 GLY	18 15N	105.3	105.34	17.327
2913 GLY	18 HN	7.944	7.94 GLU	50 HB2	1.835	1.836 GLY	18 15N	105.3	105.34	16.266

2913 GLY	18 HN	7.944	7.94 GLU	16 HB1	1.832	1.836 GLY	18 15N	105.3	105.34	5.2593
2939 GLY	18 HN	7.944	7.94 LYS	31 HN	8.673	8.664 GLY	18 15N	105.3	105.275	11.14
2939 GLY	18 HN	7.944	7.94 GLY	27 HN	8.667	8.664 GLY	18 15N	105.3	105.275	3.9221
2960 GLY	18 HN	7.944	7.939 GLU	16 HN	7.488	7.483 GLY	18 15N	105.3	105.276	3.8758
2960 GLY	18 HN	7.944	7.939 ASN	14 HD21	7.482	7.483 GLY	18 15N	105.3	105.276	6.7913
2989 GLY	18 HN	7.944	7.939 ASP	17 HN	7.144	7.138 GLY	18 15N	105.3	105.272	2.1577
2989 GLY	18 HN	7.944	7.939 ASN	14 HD22	7.14	7.138 GLY	18 15N	105.3	105.272	6.7232
3025 GLY	18 HN	7.944	7.94 ASN	14 HB1	3.026	3.016 GLY	18 15N	105.3	105.255	5.6509
3025 GLY	18 HN	7.944	7.94 ASP	19 HB1	3.011	3.016 GLY	18 15N	105.3	105.255	5.8593
3050 ASP	29 HN	9.372	9.368 ASP	29 HB2	2.531	2.522 ASP	29 15N	131.67	131.625	2.7637
3050 ASP	29 HN	9.372	9.368 ASP	36 HB2	2.521	2.522 ASP	29 15N	131.67	131.625	16.61
3050 ASP	29 HN	9.372	9.368 CYS	6 HB2	2.516	2.522 ASP	29 15N	131.67	131.625	17.754
3052 CYS	6 HN	9.201	9.201 TYR	11 HA	4.142	4.14 CYS	6 15N	131.19	131.125	4.7309
3052 CYS	6 HN	9.201	9.201 ASP	35 HA	4.135	4.14 CYS	6 15N	131.19	131.125	14.553
3052 CYS	6 HN	9.201	9.201 SER	47 HB1	4.134	4.14 CYS	6 15N	131.19	131.125	12.279
3053 CYS	6 HN	9.201	9.201 PRO	34 HA	4.168	4.175 CYS	6 15N	131.19	131.125	17.162
3053 CYS	6 HN	9.201	9.201 GLY	10 HA1	4.163	4.175 CYS	6 15N	131.19	131.125	4.0743
3057 CYS	6 HN	9.201	9.199 TYR	11 HB1	3.034	3.033 CYS	6 15N	131.19	131.125	5.2152
3057 CYS	6 HN	9.201	9.199 ASN	14 HB1	3.026	3.033 CYS	6 15N	131.19	131.125	9.5183
3059 LYS	7 HN	8.891	8.889 CYS	6 HN	9.201	9.197 LYS	7 15N	130.58	130.5	4.3816
3059 LYS	7 HN	8.891	8.889 ASN	22 HD21	9.195	9.197 LYS	7 15N	130.58	130.5	15.506
3061 LYS	7 HN	8.891	8.889 ASP	36 HB2	2.521	2.511 LYS	7 15N	130.58	130.5	17.281
3061 LYS	7 HN	8.891	8.889 CYS	6 HB2	2.516	2.511 LYS	7 15N	130.58	130.5	4.7956
3065 TRP	4 HE1	9.818	9.812 PRO	34 HB2	1.85	1.845 TRP	4 NE1	129.31	129.25	15.316
3065 TRP	4 HE1	9.818	9.812 PRO	34 HG2	1.85	1.845 TRP	4 NE1	129.31	129.25	14.417
3065 TRP	4 HE1	9.818	9.812 GLU	50 HB1	1.835	1.845 TRP	4 NE1	129.31	129.25	10.35
3065 TRP	4 HE1	9.818	9.812 GLU	50 HB2	1.835	1.845 TRP	4 NE1	129.31	129.25	9.8056
3103 ASN	25 HN	8.766	8.763 ASP	32 HB1	2.653	2.649 ASN	25 15N	127.19	127.125	8.2051
3103 ASN	25 HN	8.766	8.763 ASP	21 HB1	2.648	2.649 ASN	25 15N	127.19	127.125	10.244
3103 ASN	25 HN	8.766	8.763 ASP	21 HB2	2.648	2.649 ASN	25 15N	127.19	127.125	10.862
3106 LEU	52 HN	8.324	8.322 LYS	51 HD1	1.304	1.31 LEU	52 15N	126.74	126.75	5.5004
3106 LEU	52 HN	8.324	8.322 LYS	51 HD2	1.304	1.31 LEU	52 15N	126.74	126.75	5.362
3108 LEU	52 HN	8.324	8.319 VAL	5 HG1*	0.775	0.771 LEU	52 15N	126.74	126.75	5.362
3108 LEU	52 HN	8.324	8.319 VAL	5 HG2*	0.775	0.771 LEU	52 15N	126.74	126.75	5.362
3108 LEU	52 HN	8.324	8.319 ILE	41 HD1*	0.773	0.771 LEU	52 15N	126.74	126.75	5.362
3108 LEU	52 HN	8.324	8.319 LYS	51 HB1	0.761	0.771 LEU	52 15N	126.74	126.75	4.3935
3108 LEU	52 HN	8.324	8.319 LYS	51 HB2	0.761	0.771 LEU	52 15N	126.74	126.75	4.1337

3126 ASP	54 HN	7.829	7.827 ASP	29 HB2	2.531	2.524 ASP	54 15N	125.73	125.75	16.747
3126 ASP	54 HN	7.829	7.827 ASP	36 HB2	2.521	2.524 ASP	54 15N	125.73	125.75	28.158
3126 ASP	54 HN	7.829	7.827 CYS	6 HB2	2.516	2.524 ASP	54 15N	125.73	125.75	18.225
3130 TRP	37 HN	7.558	7.555 TYR	11 HA	4.142	4.137 TRP	37 15N	124.38	124.375	16.1
3130 TRP	37 HN	7.558	7.555 ASP	35 HA	4.135	4.137 TRP	37 15N	124.38	124.375	3.3737
3130 TRP	37 HN	7.558	7.555 SER	47 HB1	4.134	4.137 TRP	37 15N	124.38	124.375	11.878
3131 TRP	37 HN	7.558	7.554 VAL	24 HA	4.078	4.069 TRP	37 15N	124.38	124.375	9.1127
3131 TRP	37 HN	7.558	7.554 THR	28 HA	4.072	4.069 TRP	37 15N	124.38	124.375	12.764
3131 TRP	37 HN	7.558	7.554 TRP	37 HA	4.072	4.069 TRP	37 15N	124.38	124.375	2.8998
3131 TRP	37 HN	7.558	7.554 GLY	23 HA1	4.061	4.069 TRP	37 15N	124.38	124.375	10.95
3134 TRP	37 HN	7.558	7.554 ASP	54 HB1	2.54	2.534 TRP	37 15N	124.38	124.375	26.593
3134 TRP	37 HN	7.558	7.554 ASP	29 HB2	2.531	2.534 TRP	37 15N	124.38	124.375	12.802
3135 TRP	37 HN	7.558	7.558 ASP	19 HB2	2.819	2.81 TRP	37 15N	124.38	124.375	9.1353
3135 TRP	37 HN	7.558	7.558 TRP	37 HB1	2.814	2.81 TRP	37 15N	124.38	124.375	2.6053
3135 TRP	37 HN	7.558	7.558 TRP	37 HB2	2.814	2.81 TRP	37 15N	124.38	124.375	2.4143
3139 TRP	37 HN	7.558	7.544 LYS	31 HG1	1.202	1.197 TRP	37 15N	124.38	124.375	12.369
3139 TRP	37 HN	7.558	7.544 LYS	31 HG2	1.202	1.197 TRP	37 15N	124.38	124.375	11.805
3143 GLU	53 HN	8.217	8.214 VAL	5 HG1*	0.775	0.775 GLU	53 15N	122.56	122.625	15.81
3143 GLU	53 HN	8.217	8.214 VAL	5 HG2*	0.775	0.775 GLU	53 15N	122.56	122.625	15.81
3143 GLU	53 HN	8.217	8.214 ILE	41 HD1*	0.773	0.775 GLU	53 15N	122.56	122.625	15.81
3149 ILE	41 HN	8.685	8.68 TYR	11 HD1	7.312	7.311 ILE	41 15N	121.87	121.875	5.2005
3149 ILE	41 HN	8.685	8.68 TYR	11 HD2	7.312	7.311 ILE	41 15N	121.87	121.875	5.0295
3151 ILE	41 HN	8.685	8.681 PRO	40 HA	3.978	3.971 ILE	41 15N	121.87	121.875	3.4117
3151 ILE	41 HN	8.685	8.681 GLY	43 HA1	3.975	3.971 ILE	41 15N	121.87	121.875	5.2205
3151 ILE	41 HN	8.685	8.681 GLY	18 HA1	3.97	3.971 ILE	41 15N	121.87	121.875	12.395
3152 ILE	41 HN	8.685	8.673 PRO	20 HA	4.046	4.039 ILE	41 15N	121.87	121.875	12.992
3152 ILE	41 HN	8.685	8.673 ILE	41 HA	4.043	4.039 ILE	41 15N	121.87	121.875	2.967
3211 PHE	49 HN	7.744	7.736 PHE	30 HD1	6.471	6.472 PHE	49 15N	118.65	118.625	6.8459
3211 PHE	49 HN	7.744	7.736 PHE	30 HD2	6.471	6.472 PHE	49 15N	118.65	118.625	7.9258
3214 PHE	49 HN	7.744	7.738 ASP	54 HB1	2.54	2.531 PHE	49 15N	118.65	118.625	17.78
3214 PHE	49 HN	7.744	7.738 ASP	29 HB2	2.531	2.531 PHE	49 15N	118.65	118.625	13.926
3214 PHE	49 HN	7.744	7.738 ASP	36 HB2	2.521	2.531 PHE	49 15N	118.65	118.625	13.871
3215 LYS	46 HN	8.532	8.528 PRO	20 HD1	3.911	3.903 LYS	46 15N	118.16	118.125	16.497
3215 LYS	46 HN	8.532	8.528 SER	47 HB2	3.911	3.903 LYS	46 15N	118.16	118.125	5.3019
3215 LYS	46 HN	8.532	8.528 LYS	7 HA	3.892	3.903 LYS	46 15N	118.16	118.125	12.308
3217 LYS	46 HN	8.532	8.527 ASN	25 HB2	2.359	2.351 LYS	46 15N	118.16	118.125	18.597
3217 LYS	46 HN	8.532	8.527 PRO	45 HB1	2.351	2.351 LYS	46 15N	118.16	118.125	2.7057

3217 LYS	46 HN	8.532	8.527 TRP	4 HB2	2.35	2.351 LYS	46 15N	118.16	118.125	10.032
3218 LYS	46 HN	8.532	8.532 LYS	46 HB1	1.862	1.854 LYS	46 15N	118.16	118.125	2.4674
3218 LYS	46 HN	8.532	8.532 LYS	46 HB2	1.862	1.854 LYS	46 15N	118.16	118.125	3.6
3218 LYS	46 HN	8.532	8.532 PRO	34 HB2	1.85	1.854 LYS	46 15N	118.16	118.125	9.9506
3218 LYS	46 HN	8.532	8.532 PRO	34 HG2	1.85	1.854 LYS	46 15N	118.16	118.125	11.284
3222 ASP	35 HN	8.247	8.244 ASP	21 HB1	2.648	2.637 ASP	35 15N	117.66	117.625	17.073
3222 ASP	35 HN	8.247	8.244 ASP	21 HB2	2.648	2.637 ASP	35 15N	117.66	117.625	17.68
3222 ASP	35 HN	8.247	8.244 ASP	29 HB1	2.633	2.637 ASP	35 15N	117.66	117.625	13.013
3224 ASP	35 HN	8.247	8.244 ASP	35 HB2	2.486	2.477 ASP	35 15N	117.66	117.625	3.5493
3224 ASP	35 HN	8.247	8.244 ASN	14 HB2	2.479	2.477 ASP	35 15N	117.66	117.625	18.526
3224 ASP	35 HN	8.247	8.244 ILE	8 HB	2.475	2.477 ASP	35 15N	117.66	117.625	17.979
3235 ASP	32 HN	7.544	7.539 ILE	8 HG11	1.288	1.282 ASP	32 15N	116.48	116.5	17.93
3235 ASP	32 HN	7.544	7.539 ILE	8 HG12	1.288	1.282 ASP	32 15N	116.48	116.5	18.895
3236 ASP	32 HN	7.544	7.537 LEU	52 HB2	1.216	1.213 ASP	32 15N	116.48	116.5	16.088
3236 ASP	32 HN	7.544	7.537 LYS	31 HG1	1.202	1.213 ASP	32 15N	116.48	116.5	2.9282
3236 ASP	32 HN	7.544	7.537 LYS	31 HG2	1.202	1.213 ASP	32 15N	116.48	116.5	3.4143
3257 ASP	36 HN	8.089	8.086 TYR	11 HA	4.142	4.135 ASP	36 15N	114.21	114.25	18.344
3257 ASP	36 HN	8.089	8.086 ASP	35 HA	4.135	4.135 ASP	36 15N	114.21	114.25	3.3089
3257 ASP	36 HN	8.089	8.086 SER	47 HB1	4.134	4.135 ASP	36 15N	114.21	114.25	12.562
3258 ASP	36 HN	8.089	8.087 VAL	24 HA	4.078	4.068 ASP	36 15N	114.21	114.25	10.146
3258 ASP	36 HN	8.089	8.087 THR	28 HA	4.072	4.068 ASP	36 15N	114.21	114.25	13.522
3258 ASP	36 HN	8.089	8.087 TRP	37 HA	4.072	4.068 ASP	36 15N	114.21	114.25	4.732
3258 ASP	36 HN	8.089	8.087 GLY	23 HA1	4.061	4.068 ASP	36 15N	114.21	114.25	11.812
3259 ASP	36 HN	8.089	8.086 ASP	19 HB2	2.819	2.818 ASP	36 15N	114.21	114.25	11.017
3259 ASP	36 HN	8.089	8.086 TRP	37 HB1	2.814	2.818 ASP	36 15N	114.21	114.25	4.407
3259 ASP	36 HN	8.089	8.086 TRP	37 HB2	2.814	2.818 ASP	36 15N	114.21	114.25	4.5331
3266 ASP	36 HN	8.089	8.085 ASP	54 HB1	2.54	2.539 ASP	36 15N	114.21	114.25	27.937
3266 ASP	36 HN	8.089	8.085 ASP	29 HB2	2.531	2.539 ASP	36 15N	114.21	114.25	13.385
3274 GLU	16 HN	7.488	7.478 ASP	17 HN	7.144	7.139 GLU	16 15N	113.61	113.625	2.5112
3274 GLU	16 HN	7.488	7.478 ASN	14 HD22	7.14	7.139 GLU	16 15N	113.61	113.625	4.7223
3275 GLU	16 HN	7.488	7.481 GLU	16 HN	7.488	7.487 GLU	16 15N	113.61	113.625	0
3275 GLU	16 HN	7.488	7.481 ASN	14 HD21	7.482	7.487 GLU	16 15N	113.61	113.625	3.9319
3279 GLU	16 HN	7.488	7.483 GLU	48 HB1	2.219	2.216 GLU	16 15N	113.61	113.625	18.246
3279 GLU	16 HN	7.488	7.483 LYS	2 HB1	2.218	2.216 GLU	16 15N	113.61	113.625	7.6955
3279 GLU	16 HN	7.488	7.483 LYS	2 HB2	2.218	2.216 GLU	16 15N	113.61	113.625	8.6064
3279 GLU	16 HN	7.488	7.483 GLU	16 HG1	2.215	2.216 GLU	16 15N	113.61	113.625	4.1601
3280 GLU	16 HN	7.488	7.482 GLU	53 HG1	2.161	2.151 GLU	16 15N	113.61	113.625	13.628

3280 GLU	16 HN	7.488	7.482 GLU	16 HG2	2.158	2.151 GLU	16 15N	113.61	113.625	3.4007
3281 GLU	16 HN	7.488	7.483 GLU	50 HG1	2.108	2.101 GLU	16 15N	113.61	113.625	15.535
3281 GLU	16 HN	7.488	7.483 GLU	50 HG2	2.108	2.101 GLU	16 15N	113.61	113.625	16.668
3281 GLU	16 HN	7.488	7.483 PRO	20 HG1	2.094	2.101 GLU	16 15N	113.61	113.625	10.941
3282 GLU	16 HN	7.488	7.479 ASN	14 HB1	3.026	3.019 GLU	16 15N	113.61	113.625	4.6093
3282 GLU	16 HN	7.488	7.479 ASP	19 HB1	3.011	3.019 GLU	16 15N	113.61	113.625	9.2064
3283 GLU	16 HN	7.488	7.479 ASP	19 HB2	2.819	2.822 GLU	16 15N	113.61	113.625	10.12
3283 GLU	16 HN	7.488	7.479 TRP	37 HB1	2.814	2.822 GLU	16 15N	113.61	113.625	14.997
3283 GLU	16 HN	7.488	7.479 TRP	37 HB2	2.814	2.822 GLU	16 15N	113.61	113.625	14.719
3284 GLU	16 HN	7.488	7.48 TRP	4 HB1	2.617	2.618 GLU	16 15N	113.61	113.625	9.1441
3284 GLU	16 HN	7.488	7.48 ASP	17 HB2	2.617	2.618 GLU	16 15N	113.61	113.625	6.1279
3284 GLU	16 HN	7.488	7.48 ASP	35 HB1	2.617	2.618 GLU	16 15N	113.61	113.625	19.722
3284 GLU	16 HN	7.488	7.48 PHE	49 HB2	2.608	2.618 GLU	16 15N	113.61	113.625	12.819
3289 ASN	25 HD21	7.586	7.583 ASP	32 HB1	2.653	2.652 ASN	25 ND2	112.79	112.75	11.601
3289 ASN	25 HD21	7.586	7.583 ASP	21 HB1	2.648	2.652 ASN	25 ND2	112.79	112.75	11.885
3289 ASN	25 HD21	7.586	7.583 ASP	21 HB2	2.648	2.652 ASN	25 ND2	112.79	112.75	11.915
3357 GLY	18 HN	7.944	7.937 PRO	40 HA	3.978	3.971 GLY	18 15N	105.3	105.25	12.969
3357 GLY	18 HN	7.944	7.937 GLY	43 HA1	3.975	3.971 GLY	18 15N	105.3	105.25	16.539
3357 GLY	18 HN	7.944	7.937 GLY	18 HA1	3.97	3.971 GLY	18 15N	105.3	105.25	2.3017
3359 GLY	18 HN	7.944	7.939 TRP	4 HB1	2.617	2.617 GLY	18 15N	105.3	105.25	9.4068
3359 GLY	18 HN	7.944	7.939 ASP	17 HB2	2.617	2.617 GLY	18 15N	105.3	105.25	3.9354
3359 GLY	18 HN	7.944	7.939 ASP	35 HB1	2.617	2.617 GLY	18 15N	105.3	105.25	17.853
3359 GLY	18 HN	7.944	7.939 PHE	49 HB2	2.608	2.617 GLY	18 15N	105.3	105.25	12.687