**Programming Assignment**

For this assignment, submit two programming files, one for each problem. You must also submit two figures, one of the Ramachandran plot of valine and one showing the observed and calculated χ1 distribution.

**Problem 1**

Ramachandran plots allow us to investigate the sterically allowed and disallowed backbone dihedral angle combinations φ and ψ in proteins. Using the file *Val\_residues.txt* provided, produce a Ramachandran plot for valine residues. The file *Val\_residues.txt* contains 1000 valine dipeptides taken from a database of high-resolution protein crystal structures. The data for a representative valine dipeptide is shown in Table 1. The Cα, caroboxyl carbon, and oxygen atoms on the prior amino acid are labelled pCa, pC, and pO. The N, Cα and H atoms on the subsequent amino acid are labeled: nN, nCa and nH. Using this file, calculate φ and ψ for each residue and produce a Ramachandran plot similar to that shown in Figure 1.



α

Figure 1: Ramachandran plot for 1000 valine residues. The Ramachandran limits for α-helices and β-sheets are shown in blue.

β

**Problem 2**

The hard sphere model assumes that atoms in proteins interact only via steric repulsion. The file *Val\_rotated.txt* contains the coordinates of one Val dipeptide as it is rotated around its side chain dihedral angle, χ1. The dihedral angle is specified in column 1. Using this data, calculate the repulsive Lennard-Jones energy (which approximates the hard-sphere potential in the low-temperature limit) for each side chain conformation using Equation 1 below:

(1)

where is the center-to-center separation between atoms *i* and *j*, is the Heaviside step function, is the energy scale of the repulsive interactions, = /2, and is the radius of atom *i.*

In this equation, assume = 1. The Heavyside step function sets U = 0 when the atoms are not overlapping The atomic radii, in Å, are listed in *Val\_radii.txt*. The total energy URLJ(χ1) should be calculated between all non-bonded pairs involving side chain atoms. For example, the energy should be calculated between Cg1 and N but not between Cg1 and Ca.

The total energy URLJ(χ1) can be converted into a probability distribution using , where *kBT/ε* = 0.01 and A is a normalization constant so that . Plot the predicted probability distribution and compare it to the distribution observed in high-resolution protein crystal structures. You should generate the observed distribution from the file discussed in Problem 1. The observed distribution should be similar to that shown in Figure 2.

Table 1: Atom labels and coordinates for the first Val dipeptide in Val\_residues.txt



Macintosh HD:Users:jennifergaines:Documents:Val_observed.eps

Figure 2: The side chain dihedral angle distribution P(χ1) for Val observed in high-resolution protein crystal structures.

Non-Programming Assignment

**Problem 1**

Derive the expressions for the x-, y-, and z-components of the force on atom j=i+1 from the previous atom i and successive atom k=i+2 using the bond angle potential, , where kθ is the constant bond stiffness, is the bond angle between bonded atoms i, j, and k, , and θ0 is the preferred bond angle. Note that .