Biophysical Chemistry Assignment

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For calculating the torsional angles of a polypeptide chain our code starts by taking a pdb file as input and opening that file. This file is then read line by line and data corresponding to the line starting with “ATOM” are stored in a matrix.

From the matrix three atoms are taken from each amino acid considering them in a chain vectors are formed. Taking these vectors normal are calculated for the three plains for each psi and phi angles.

From these normals sin and cos of the angle between the vectors are calculated and then for getting the angle with sign the function atan2d() was used and the psi and phi angles were stored with sign in an matrix.

The final output returned by the function is a matrix which contains psi and phi angles respectively in a matrix starting from N terminal.