CS150 - Assignment 1
(100 pts)
Due date: TBD

Purpose:
Get familiar with PDB format; know how to process pdb files and retrieve needed information; perform geometric calculations and manipulations of the structure.

Helpful links:
Using PDB
PDB: www.rcsb.org
Understanding PDB data: http://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data
PDB file format: http://www.wwpdb.org/documentation/file-format-content/format33/v3.3.html
PDB at Europe: www.pdbe.org
They are many nice online training courses at PDBe: http://www.ebi.ac.uk/training/online/

Visualization software:
Rasmol: http://www.openrasmol.org/
Pymol: www.pymol.org

Programming languages for the assignment: any. However, some languages may work better than others.

Assignment Description:
Search and download 2GB1.pdb from PDB website (www.rcsb.org)
Your program should be able to do the following:

1. (10 pts) read the pdb file and retrieve the coordinates of the backbone atoms (specifically those of N_i, CA_i, and C_i.)
2. (30 pts) calculate and output the mean and std (standard deviation) for each of the following variables:
    a. bond lengths: N_i-CA_i, CA_i-C_i, C_i-N_{i+1}
    b. bond angles: N_i-CA_i-C_i, CA_i-C_i-N_{i+1}, C_i-N_{i+1}-CA_{i+1}
    c. distance between adjacent CAs, i.e., between CA_i and CA_{i+1}
3. (30 pts) For residue 30, which is a Phenylalanine, compute and output its torsional angles: phi, psi, and omega.
4. (30 pts) Now set both phi and psi angles of residue 30 (Phenylalanine) to 0 degree. Note this will change the coordinates of many residues.
    a. (20 pts) Recompute the coordinates of all the residues (including their side chain atoms). Use the new coordinates to replace the old and construct a new pdb file called 2GB1-new.pdb (everything else in the file should stay the same).
    b. (10 pts) Is there any steric clashing now that the phi and psi angles of Phenylalanine 30 are set to be 0? What is the minimum distance between atoms in the current structure? Identify the pair of atoms that have the minimum distance. Please identify each atom by its type and its residue number and type. For example, CA of Ala 15, N of GLY 16.

5. (Bonus: 25 pts) Extend your program so that it can compute the side chain torsional angles (χ's). Apply your program to 2GB1.pdb and output the side chain χ angles of each residue.

Submission:
when you are finished and ready to submit, put your program, 2GB1-new.pdb, and a text file that contains all the output (which should be easy to understand) into a folder called hw1*yourLastName*. Zip up the folder into hw1*yourLastName*.zip. *Don't use other archivers than zip.* Then upload it to the HW1 assignment on Canvas.

For this assignment, you can either work alone or form teams of 2. If so, only one submission per team is needed.