BIO INFORMATICS

REPORT ON PROJECT

Task-1:

INPUT : PDB file

OUTPUT : My program outputs on the console. Outputs the beginning and ending amino acid indexes of each β-strand along with the vector of a β-strand.

Below is the screenshot of my program for 1S04.pdb. You can test with other pdb files.

```
C:\Users\sindhuja>cd..

C:\Users>cd..

C:\>cd python34

C:\Python34>cd BIO PROJECT

C:\Python34\BIO PROJECT>python task1.py
Enter input file name: 1S04.pdb
NAMES:  TRP MET
Indices:  ('3', '5')
Vector:  ['-13.469', '1.179', '4.489'] ['-12.361', '0.148', '-2.201']
NAMES:  ILE PHE
Indices:  ('40', '42')
Vector:  ['-10.937', '-2.344', '4.272'] ['-12.064', '-4.422', '-1.684']
NAMES:  LEU ALA
Indices:  ('47', '53')
Vector:  ['-9.995', '-8.779', '-0.570'] ['-0.056', '0.602', '11.672']
NAMES:  GLU GLU
Indices:  ('104', '106')
Vector:  ['1.014', '-1.696', '6.602'] ['-2.715', '-7.368', '6.319']

C:\Python34\BIO PROJECT>
```

Task-2:

INPUT : PDB file

OUTPUT : Outputs the aligned β-strands in PDB format using new position for each β-strand. It contains the line of SHEET and the corresponding lines with ATOM new coordinates of (x, y,z) for each atom on the strand.

HOW TO RUN MY CODE FOR TASK-2 :

Install numpy library for python on your computer.

I used this because it supports for large arrays, matrices and for calculating any mathematical functions.

Run the code. It prompts the user to enter the name of pdb file. Input the name of any pdb file.It then generates the final.pdb file in the folder where you have the code. Place the final.pdb file in chimera to see the alignment.

BRIEF UNDERSTANDING OF CODE:

The program in task1 already gets the start and end coordinates of each beta strand.

We then find the strand we want all the other strands to orient themselves with, and use the start and end of that as the start1 and end1 parameters.

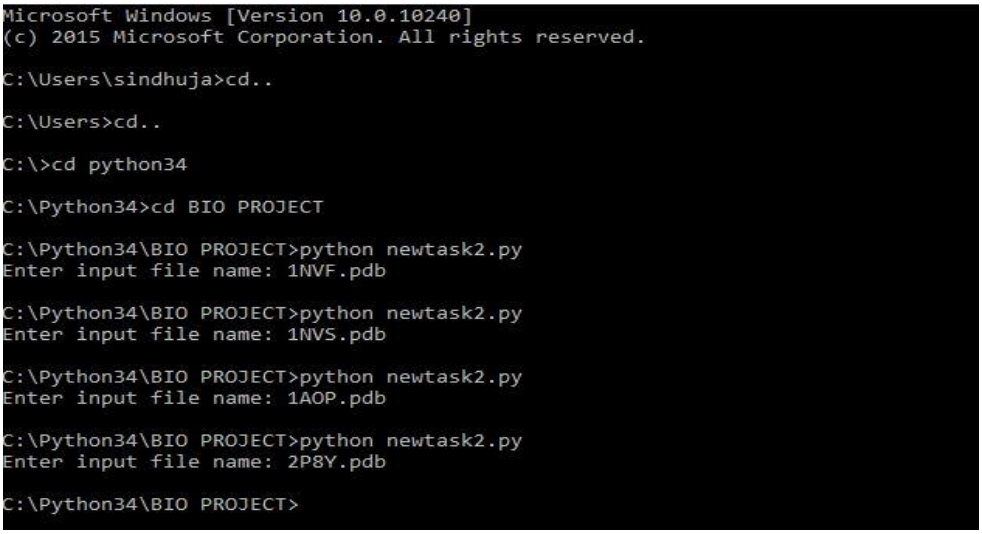
We then call transform_vector once for each other strand, passing the start and end of the vectors of each other strand as start2 and end2.

Returned will be a tuple with two elements, each of which is a 3D point.

We then write these points out as the new coordinates of the alpha-carbon in the PDB file.

Below is the screenshot for task2:

I tested it for all the files as shown in screenshot:



Below is the screenshot of the alignment for 1NVS.pdb in chimera.