

IDC306: Biocomputing  
Assignment-5  
Date: 27 Feb 2024

Instructions:

- a. Do not use any package or module to read PDB file.
- b. Do not use ChatGPT.

RESID: 23-26  
RESNAME:18-20  
ATOMNAME:12-16  
Xcord: 31-38  
Ycord: 39-46  
Zcord: 47-54  
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Q1. Write a program to read the content of the PDB file into the dict data type in the following form:

```
x[RESID][ATOMNAME]=[Xcord,Ycord,Zcord]
```

```
x[RESID]['resname']=RESNAME
```

for instance, using `x[5]['resname']` should return residue name and `x[5][CA]` should return list with coordinates.

Q2. After reading the content, the program should be able to do the following:

- a. Find the composition of the residues. (occurrence of amino acids in the PDB file).
- b. Find whether a residue has the same number of atoms. Find the average number of atoms.
- c. Find the average distance between two consecutive CA residues using the formula:

$$v1=[x1,x2,x3] \text{ and } v2=[y1,y2,y3]$$
$$vdiff=v2-v1 \text{ (vector difference)}$$
$$d=\sqrt{vdiff.vdiff}$$