Report

β-strands

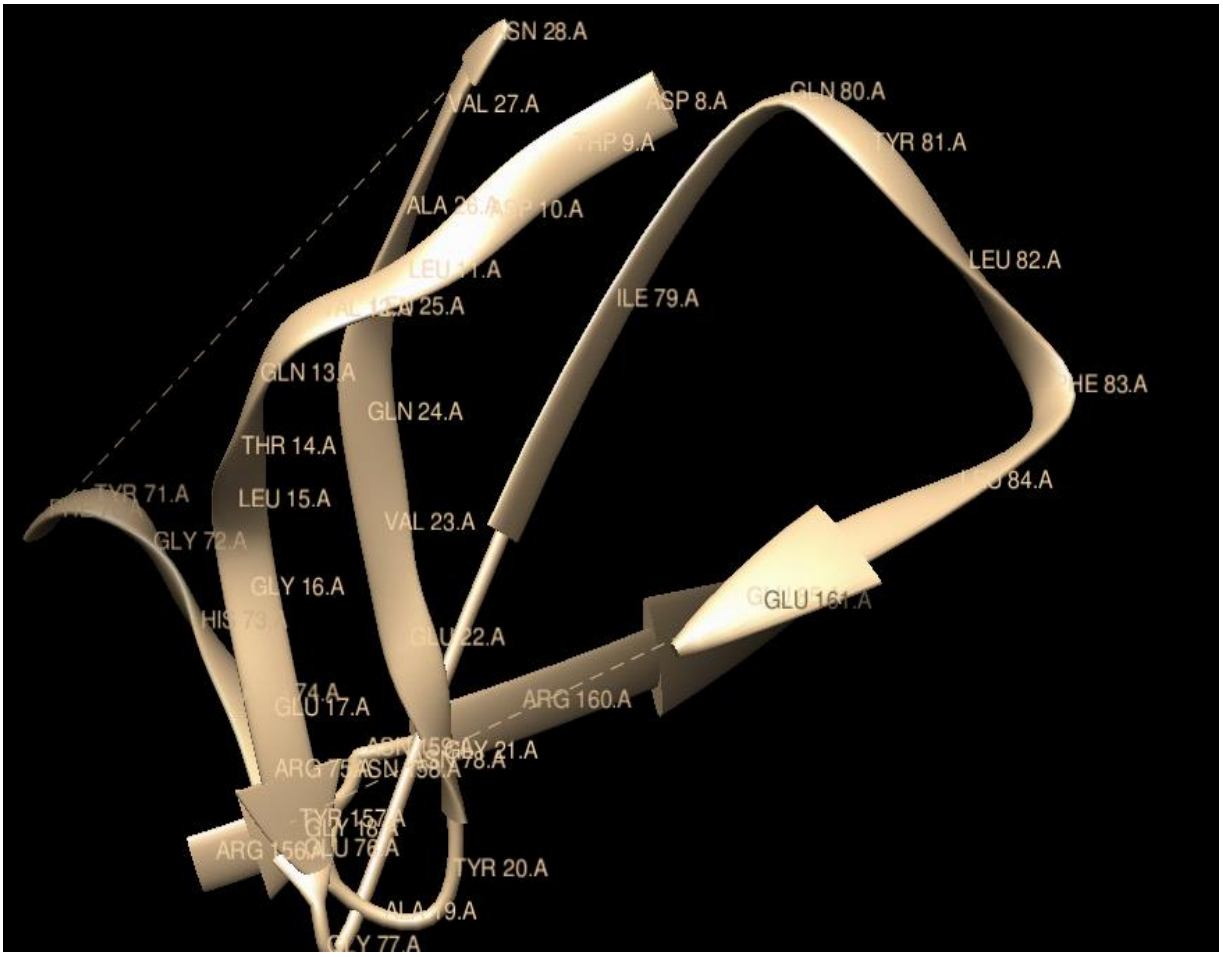
A protein structure is represented using PDB format that is a text file with annotation of structure details. You can find the definition of PDB format in Protein Data Bank (pdb.org) website. β-strands are portions of a protein chain responsible for forming β-sheets. They can be recognized in a PDB file from the lines beginning with "SHEET".

Program:

For rotation and alignment program is written in C++. The input data considered is the atoms data for the sheets that are extracted (in Task-1). Considered data for testing is 1NVS.pdb

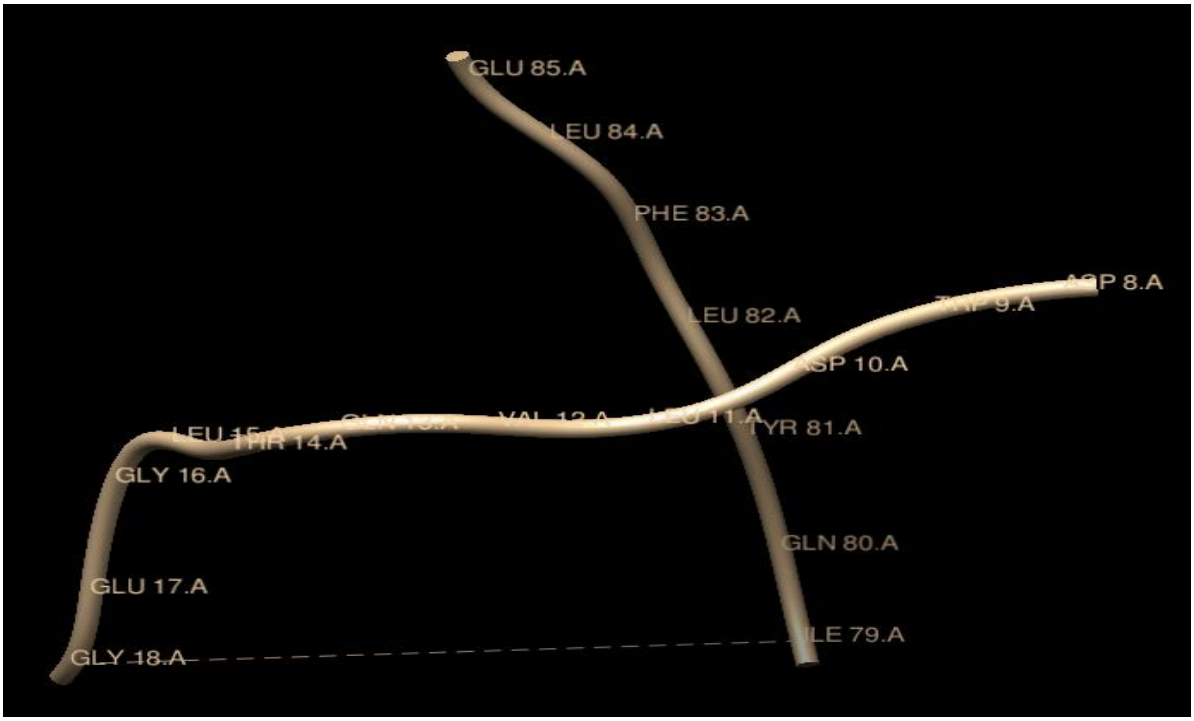
The instructions to run the program is mentioned in the Readme file that is included in the Project folder.

The output obtained when viewed using chimera is as below:

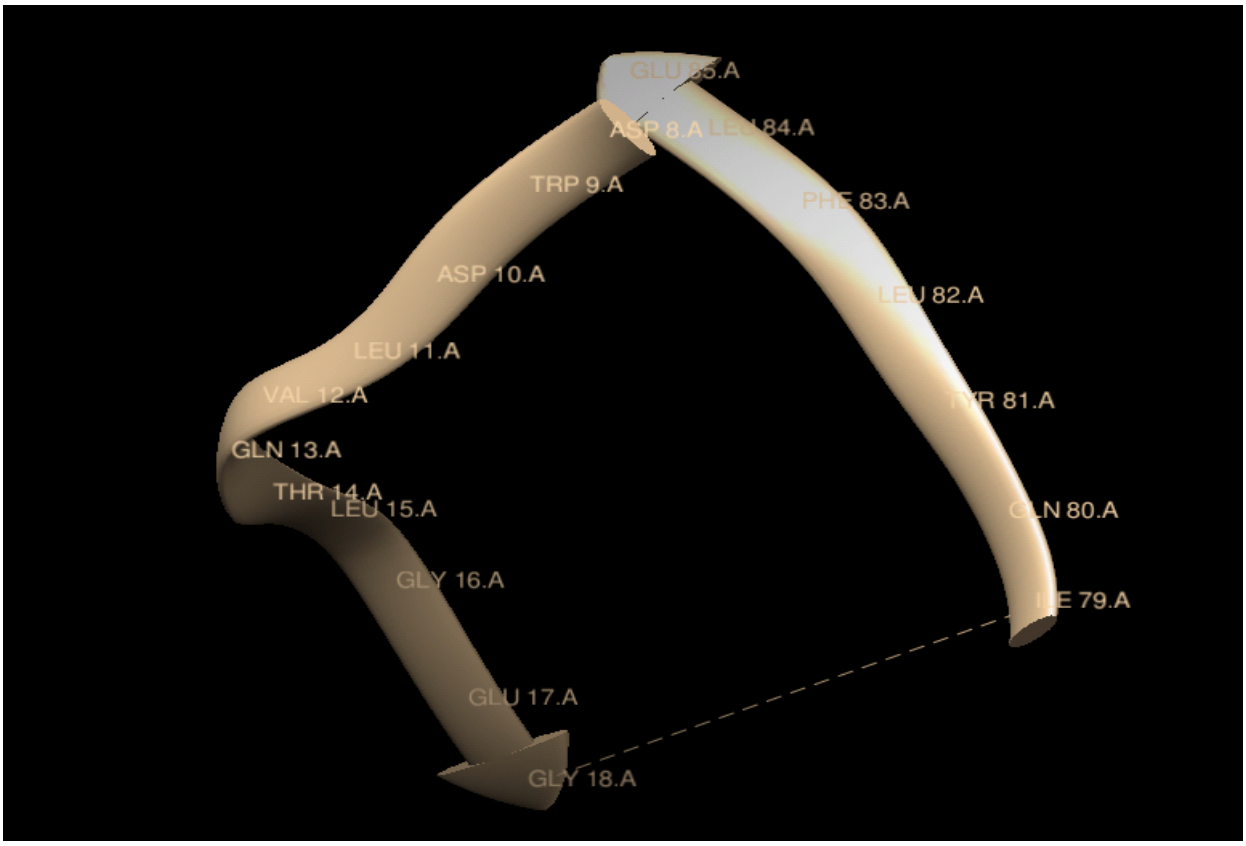


The vector considered is the first C-Alpha atoms of the sheet. In the below picture the considered vector is Atoms 8, 9 and 10 and another vector is Atoms 79, 80 and 81.

Before alignment and rotation:



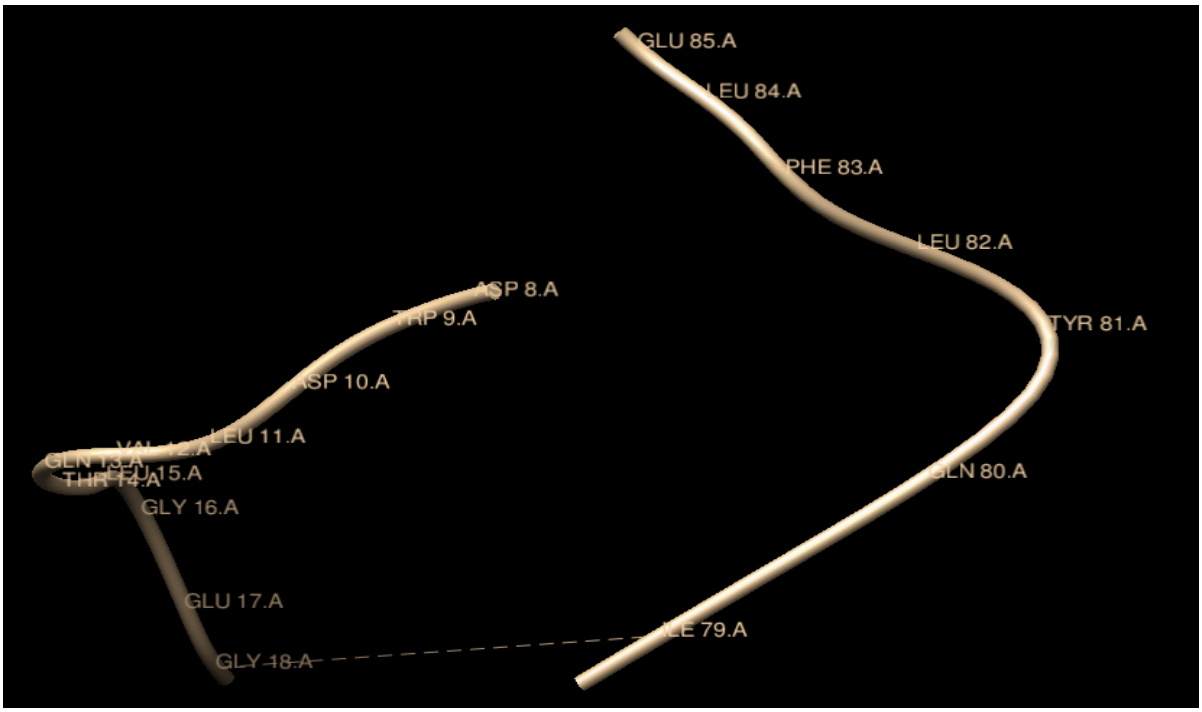
Specifically for report and better understanding I have removed the other extra data. The output contains the whole Atoms and Sheet data.

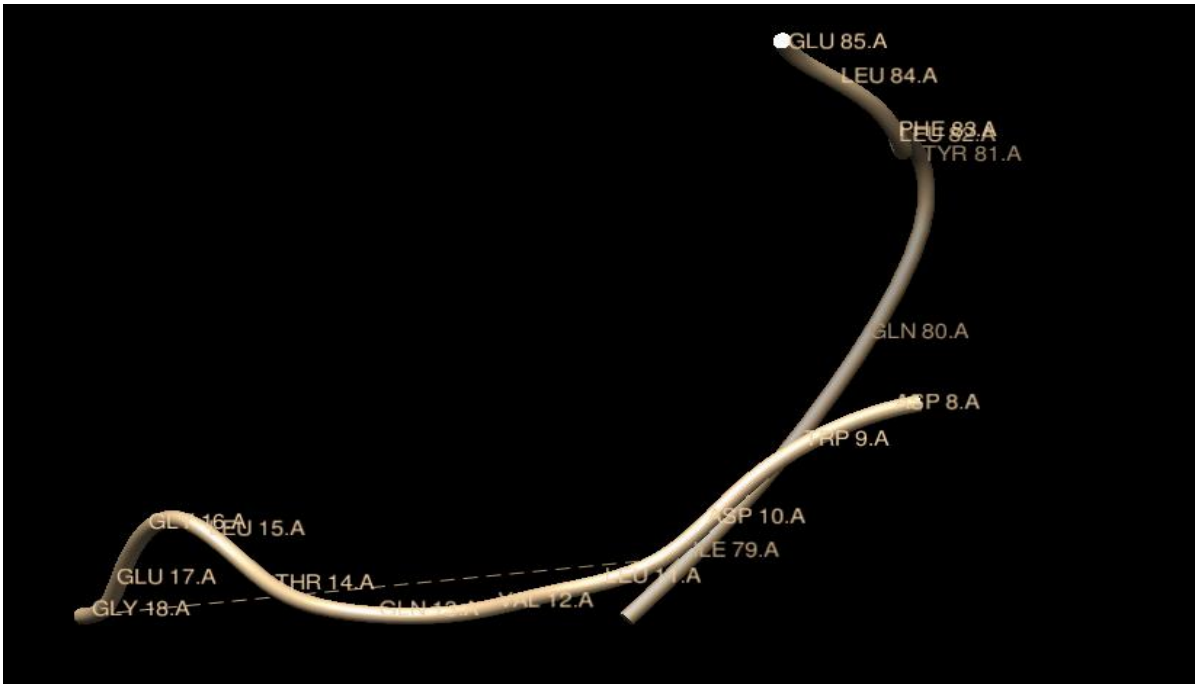


In the picture above the two vectors are perpendicular to each other initially.

After alignment and rotation:

The two vectors are aligned by rotating the vector with Atoms 79, 80 and 81. Below are the snapshots from the chimera, the two views of the output from the program.





The above snapshot is another view of the aligned vectors.