Title: Detecting knots and slipknots in protein chains.

Proteins are fundamental entities of all biological creatures. They are made up of chains containing large number of amino acid residues. The structure of the protein chain affects energy of the protein structures. Protein chains very rarely have knots and even rarely have slipknots. They should generally be avoided in protein models, as they make it a complicated to reach the native state. This project deals with finding and visualizing knots and slipknots in the protein structures. Knots in the protein chains are any structures in which the chain goes through a loop of residues and is tied up. However, slipknots are a type of knots in which the polypeptide chain goes through a loop and eventually the knot vanishes as the chain double backs on itself. These types of knots are generally not detected in the knotfind algorithms.

This project uses and expands the knotfind algorithm which simplifies the entire polypeptide chain by considering three consecutive atoms (i-1, i, i+1) and check if there is a intersect cutting through it, if no intersect cuts through the triangle formed by those three atoms then the i’th atom is pruned and the next set of atoms are considered. If a intersect is found the i’th is skipped and the next set is considered and this process is repeated until all the atoms are considered. Knotfind algorithm then outputs k3 and k2 atoms which are the starting and the ending atoms of the knot and then a PDB file which has the un simplified atoms that were found in the knotfind along with N and C terminals. The slipknotfind algorithm however first finds the knot and run the knotfind algorithm iteratively until the knot which was earlier detected vanishes, the atom which unties the knot is called the k1 atom and the three atoms k3, k2 and k1 are reported along with a PDB file which contains the un simplified atoms in the chain. The resulting PDB files are then visualized with PyMol a tool which is often used to visualize protein structures. Along with it we also have a Python script which explains the visualization better by highlighting the knotted regions of the protein.

This project can further be developed by making it available on the internet and modifying it to run on a server which can enable the biochemists around the world to test and make sure that their samples are not knotted/slipknotted and also run this algorithm on plethora of protein structures to discover knots and slipknots in them which were not reported earlier.