

Title: Detecting and visualizing knots and slipknots in protein chains.

Abstract

Proteins are made up of chains containing a large number of residues and are fundamental entities of all biological creatures. Protein chains very rarely have knots or slipknots and these should generally be avoided when predicting protein structures, as they make it more difficult to reach the correct fold. This project focuses on finding and visualizing knots and slipknots in protein structures. A protein is said to be knotted if the chain loops through itself and not back out again through the same loop. Slipknots occur when the polypeptide chain goes through a loop but the chain eventually doubles back on itself, removing the knot. As slipknots are not mathematically knots, the standard protein knot detection algorithms do not report them.

In this project we improve one such knot detection algorithm, Knotfind, to find slipknots in proteins and we have established a server for everyone to use. Our new algorithm iteratively searches subsections of a protein chain and checks each of them for knots. If a knotted region is found, we search for the residue that unties the knot resulting in a slipknot. In order to visualize the knotted or slipknotted region, our algorithm generates a simplified protein chain stored in a text file that is loaded using JSmol (a Java/HTML5 based molecular visualization tool). Using the JSmol API we then highlight the slipknotted region of the protein chain, along with the residues that untie the knot, clearly defining the slipknot.