

Lab Assignment 0: foldIt

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The first noticeable phenomenon is clashing which appears when two atoms are very close to each other, almost occupying the same space, and since this is not feasible it presents a bad configuration. On the other hand, voids appear when atoms are very far apart causing the protein not to be closely packed. Hydrogen bonds play an important role, since they yield a lower energy configuration. We find these bonds between sheets, along helices, and sometimes with sidechains. Two particular groups of sidechains are hydrophobic and hydrophilic ones. The hydrophobic ones tend to fold towards the inside of the structure. Hydrophilic chains might form weak bonds with the outside, creating a balance in this way. Hydropathy represents the number of hydrophilic or hydrophobic properties of an amino acid sidechain. Other relevant type of bond is the disulfide bond, which occurs between two cysteine chains. One last point that was noted, was the type of loop that connects secondary structure, which is dictated by the amino acid chain that binds the structures and determines structural folding properties.

