Chemistry of Life

Types of atoms and chemistries in biological macromolecules

Biological macromolecules include proteins, nucleic acids, and polysaccharides. We will emphasize proteins and nucleic acids because they are key biopolymers for which there are extensive structural data.

The major types of atoms in biopolymers are carbon, nitrogen, oxygen, phosphorus, sulfur, and hydrogen. Other atoms, such as iron, zinc, calcium, are important components of some proteins or protein-ligand complexes. Conventionally for the display of structures **nitrogen atoms are colored blue, oxygen atoms are red, and sulfur and phosphorus atoms are yellow**.

Individual atoms are connected by strong covalent bonds to form molecules. The molecules fold into three-dimensional shapes by means of electrostatic forces. Noncovalent bonds or interactions (ionic, hydrogen bond and van der Waals) describe the interactions within molecules that stabilize the three-dimensional fold and the interactions between molecules in a complex. These interactions occur between different parts of a macromolecule, between two macromolecules e.g. protein-RNA, and between a macromolecule complexed with a small ligand.

See notes at: users.rcn.com/jkimball.ma.ultranet/BiologyPages/B/BondEnergy.html
users.rcn.com/jkimball.ma.ultranet/BiologyPages/N/Noncovalent.html
users.rcn.com/jkimball.ma.ultranet/BiologyPages/H/HydrogenBonds.html

Types of Interactions:

1. **Covalent Bond**
   (Strong and Irreversible)

2. **Ionic or Salt Bridge**

(A positively charged group about 3-4Å from a negatively charged group, e.g., Arg +....- Asp)

Electrostatic energy = $q_1 \times q_2 / r$

3. **Hydrogen bond**

(A hydrogen bond donor and acceptor separated by 2.7-3.3Å, e.g., C=O....H-N)

4. **Hydrophobic or van der Waals**

(Non-hydrogen bonding atoms separated by the sum of their van der Waals radii - about 3.5Å, e.g., C-H....H-C)

Parameterize the hydrogen bond and van der Waals interactions using a Lennard-Jones potential with Attractive term of $-a_1a_2/r^6$ and Repulsive term of b_1b_2/r^{12}

(These are empirical definitions from atomic structures)