

How Do Amino Acids React to Water and Oil?

What are the forces on side chains (or residues) of amino acids when they are in water?

When amino acids are joined together in proteins, only their side chains (also called radicals or residues) are left free to interact with each other and molecules of their surrounding medium (water or lipids). These side chains, therefore, have a strong influence on how the protein behaves in water.

There are three forces at play between amino acids when they are not in water:

1. **Van der Waals forces**: the natural stickiness of each individual atom, caused by the movement of its electron cloud. While small, this effect can be substantial when two molecules can line up close to one another.

2. **Electrostatic charge**: the ions of a side chain that have either plus or minus charge. In a charged side chain, an atom has either lost an electron and become a positive ion or gained an electron, and becomes a negative ion.

3. **S-S bonds**: Several sulfur (S) - containing amino acids, such as cysteine, located in the different parts of the protein chain, interact with each other, making covalent bonds that link two different parts of a protein molecule together. They often form loops in the otherwise straight chains. Every S-S bond made between two molecules of cysteine serves as a "staple" holding the shape in a more steady position. (See the S-S bond in Fig. 2) This covalent bond is not as strong as the peptide bond between amino acids, and breaks when heated, though at a temperature lower than that required to break the peptide bonds making the protein chain.

BUT when proteins are in water, water molecules add yet another force resulting from the polar nature of water molecules:

4. **Hydrogen bonds**: Because the water molecule's oxygen is strong, it pulls the

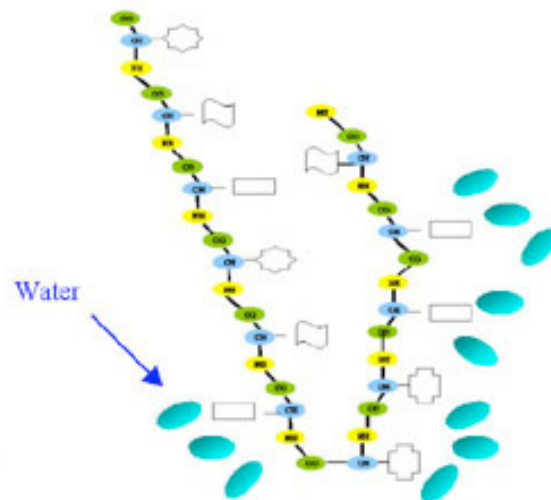


Fig. 1 A protein fragment. Water-fearing amino acid side chains are herded into the center of the protein. Water is found outside the protein, where "water-loving" side chains are attracted to the polar water.

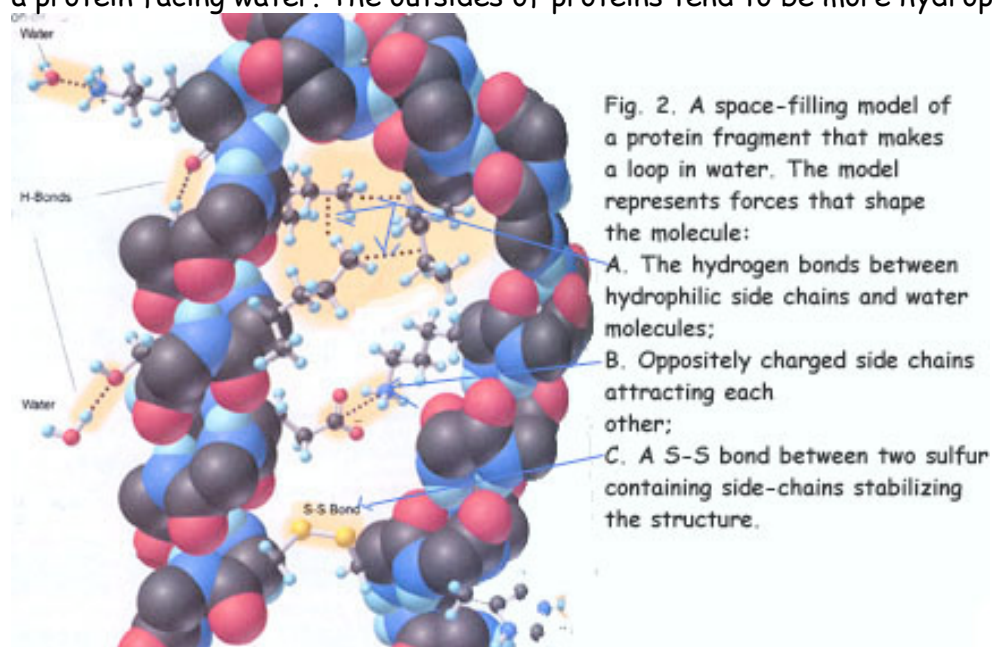
electron cloud away from its two hydrogen, making its hydrogen slightly positive and therefore capable of interacting with negative poles on neighboring molecules.

*Hydrogen bonds are really a form of electrostatic charge, but weaker than the charges on most ions. Because the influence of water molecules is so important, a hydrogen bond is called by a separate name.

Hydrophilic ("water loving") amino acid side chains are either charged or polar (with separated plus and minus charged areas). Both are attracted by water molecules.

Unlike the charged side chains, polar side chains are overall neutral, but still capable of attracting water to places on their surface. They neither gain nor lose an electron but simply shift the electron towards one of the atoms. Such a polar side chain remains neutral as a whole, but the separation of the "pluses" and "minuses" within it creates two opposite "poles", each capable of attracting water molecules.

The part of the protein that is rich with amino acids having charged or polar side chains is pulled away by polar water molecules into a protrusion on the surface of a protein facing water. The outsides of proteins tend to be more hydrophilic than the inner areas.



Hydrophobic ("water-hating") amino acid side chains are electrically neutral and non-polar in relation to water. They do not lose or gain electrons, and do not have shifted electrons.

Neutral, non-polar amino acids are just as important in the shaping of a protein as charged or polar ones. Because they do not bond with polar water, they tend to be

herded together on the inside of molecules, appearing to avoid water as much as they can. The core of molecules therefore tends to be neutral, a "hydrophobic core." These "water-fearing" molecules also tend to avoid contact with the hydrophilic charged and polar side chains in the protein. The water around them instead tries to make as many bonds with other nearby water molecules as possible, effectively herding non-polar amino acids towards other non-polar amino acids.

How do side chains interact with lipids (all fats, including oil)?

Hydrophilic amino acids (charged and polar) will respond in a way that is opposite from their response to water. When placed in oil, they will be more attracted to **each other** than to the surrounding molecules. **Non-polar, hydrophobic amino acids** will not be "herded together" by the oil, as they were by water, so they will effectively dissolve.

Impacting the Shape of a Protein

The position of ALL amino acids in the chain dictates the shape of a protein. Moreover, their position in the chain defines how far, for example the charges are from each other, or where the hydrophobic "dent" or hydrophilic "bump" on the protein's surface will occur.

A Simplified Model. In our model the structure of the amino acids has been simplified, simply represented as beads along a peptide chain. These beads are linked to each other with covalent bonds, and each is assigned a property which reflects how hydrophobic or hydrophilic it is.