



IIT Guwahati

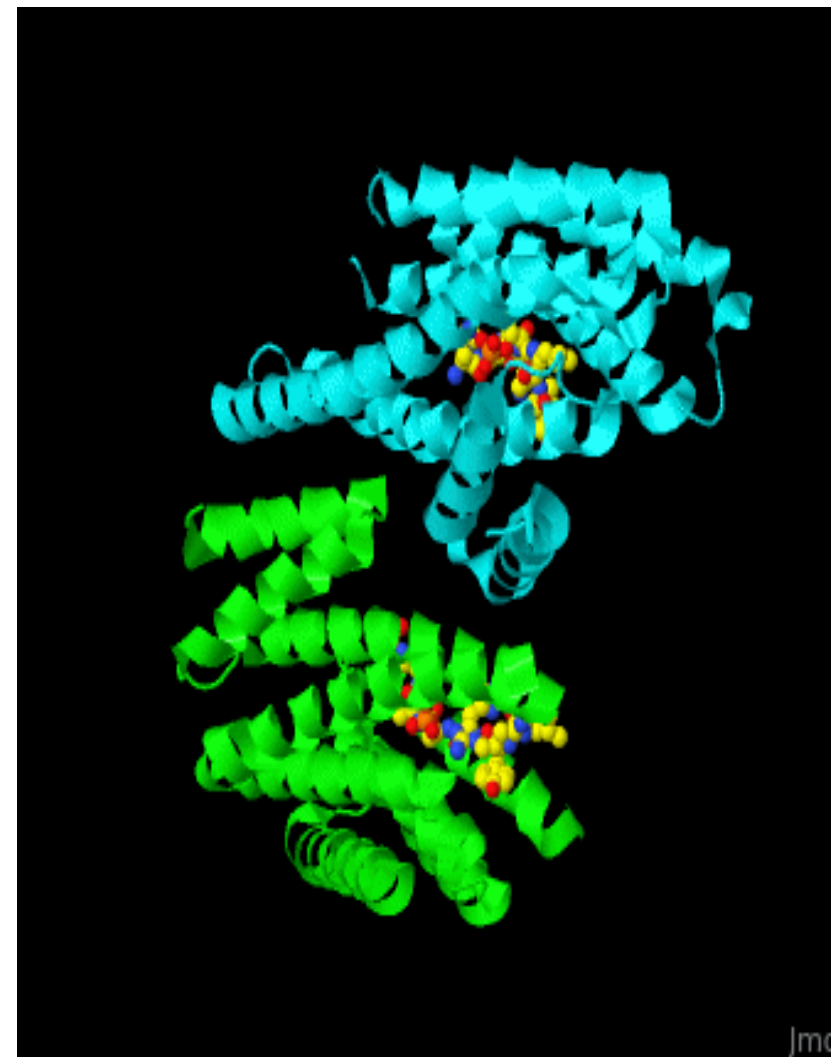
Lecture 15

Course BT 631

Protein Structure function and Crystallography

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Interactions that stabilize tertiary structure

3. Electrostatic (Charge-charge) or Ionic interactions

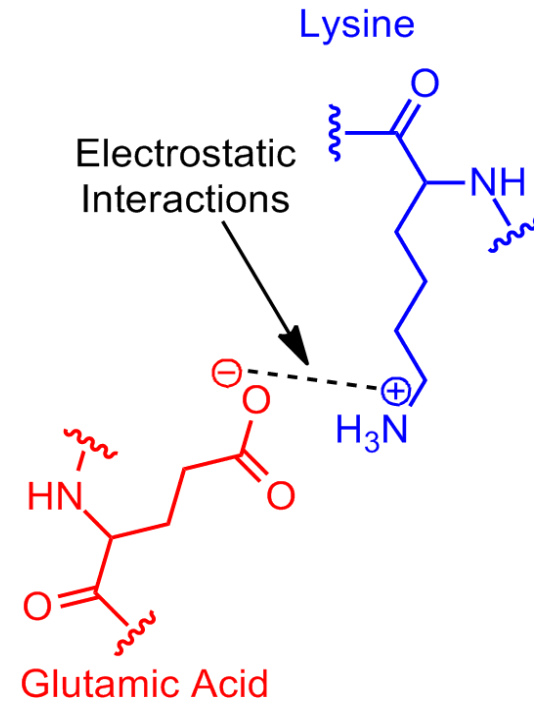
These interactions occur between the side chains of oppositely charged residues as well as between the Amino and Carboxyl groups at the ends of polypeptide chains.

The side chains of Lys, Arg and His together with side chains of Asp and Glu and to lesser extent Tyr and Cys are involved in **Charge-charge interactions**. These forces can be determined by Coulomb's law,

$$V = q_1 q_2 / \epsilon_0 4\pi r^2$$

V is Potential energy between two charges, q_1 and q_2 are magnitude of charges, r is separation distance between these charges and ϵ_0 (**Epsilon**) is the permittivity of the medium (water) and is related to dielectric constant (ϵ_r) by

$\epsilon_r = \epsilon / \epsilon_0$ where, ϵ is the permittivity of the space.

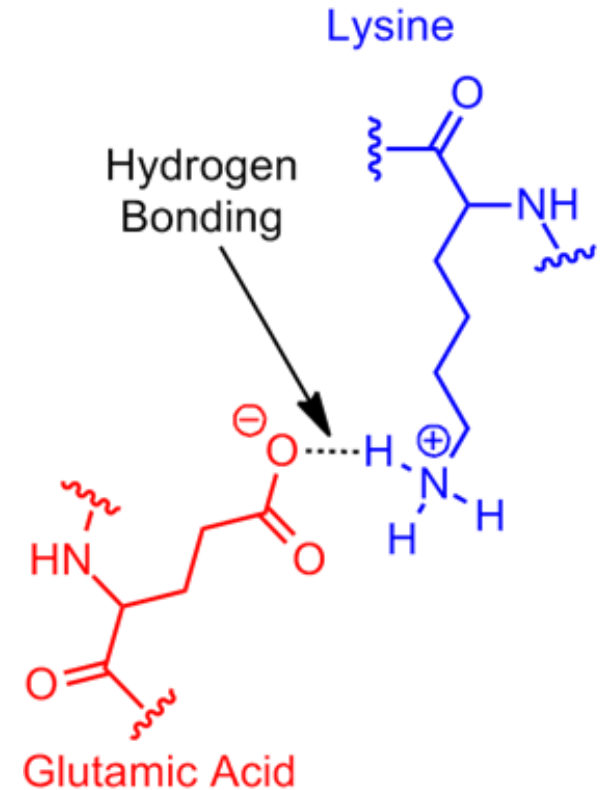


Ionic interaction between (+)charge of NH₂ group of Lys and (-)charge of Carboxyl group of Glu.

Interactions that stabilize tertiary structure

4. Hydrogen Bonding

- The polypeptide chain fold can form H-Bonds between the side-chain groups as well as between the main-chain and side-chain groups.
- **Hydrogen bonds contribute significantly to the stability of α -helices and to the interactions of β -strands to form parallel or anti-parallel β -sheets. These H-bonds provide overall stability to the tertiary structure or the folded state.**
- H-bonds vary in length from 0.26 to 0.34 nm. This is the distance between the heavy atoms, between N and O in Hydrogen bond of the type N-H ---- O=C and may deviate in linearity by 40° .
- **Side chains of Tyr, Thr, Ser containing OH group and side chains of Gln and Asn with amide group are important in H-bond formation.**

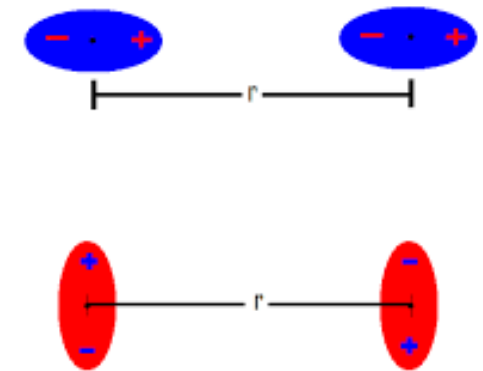


H-Bond between NH_2 of Lys and Carboxyl group of Glu.

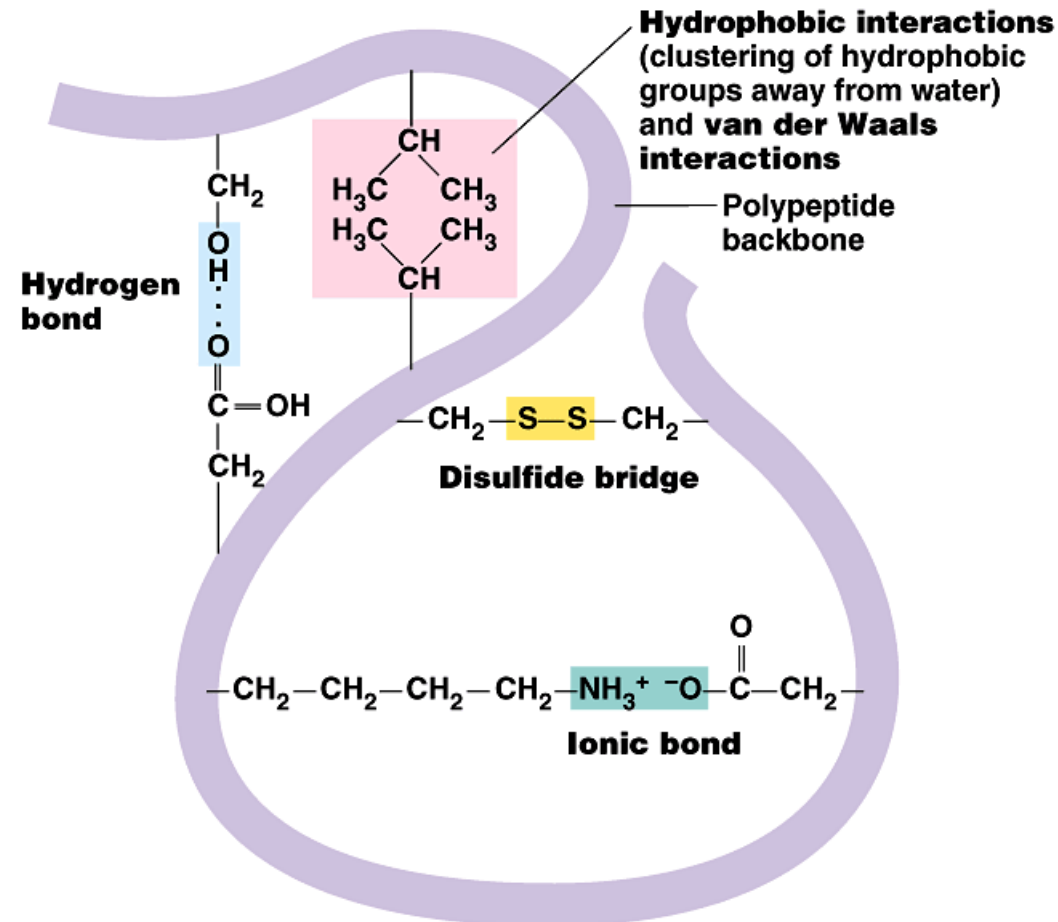
Interactions that stabilize tertiary structure

5. van der Waals interactions

- These interactions occur between the adjacent, uncharged and non-bonded atoms and arise from the induction of dipoles due to fluctuating charge densities within the atoms. Since atoms are continuously oscillating the induction of dipoles is a constant phenomenon.
- There are attractive and repulsive van der Waals forces that control interactions between atoms and are important in protein folding.
- Unlike electrostatic interactions these induced dipoles do not follow Coulomb's law and they vary in their contributions to the overall intermolecular attraction.



Interactions that stabilize tertiary structure



A protein's folded state reflects the summation of disulfide bridges, Hydrogen-bonding, hydrophobic, electrostatic and van der Waal's interactions.

Interactions that stabilize tertiary structure

Bond energy for interactions between atoms in Proteins

Interaction	Bond energy (kJ/mol)
Covalent	~200
Electrostatic	<20
Hydrophobic	<10
Hydrogen Bonding	<10
Van der Waals	<5