IIT Guwahati

Lecture 8

Course BT 631

Protein Structure function and Crystallography

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Structure of Protein

Secondary Structure

- It is defined as local spatial arrangement of the polypeptide chain.
- Secondary structure is the initial folding pattern (periodic repeats) of the linear polypeptide.
- The three basic units of secondary structure are α-Helix, the β-Strands and turns. All other structures represent variations of one of these basic themes.

Types of Secondary Structure

A) Regular Secondary Structure

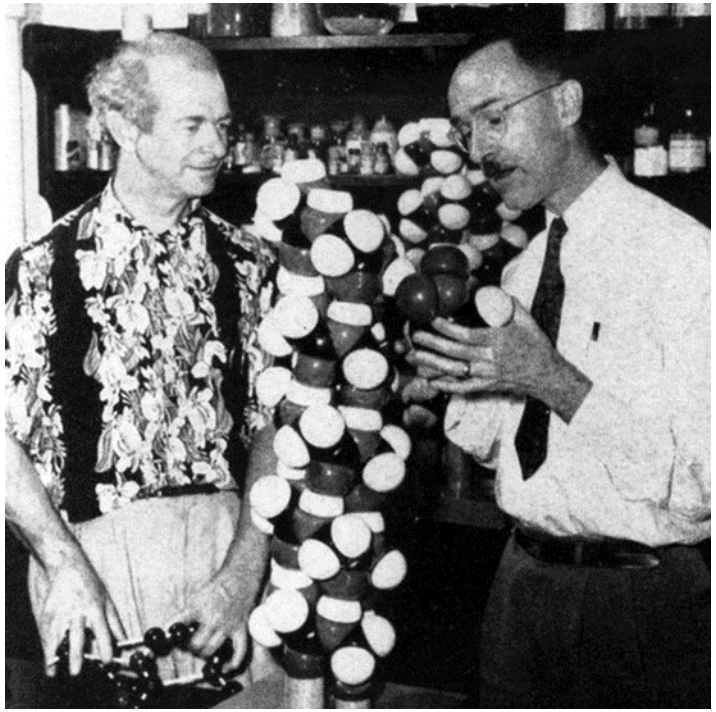
B) Irregular Secondary Structure

A) Regular Secondary Structure

Regular Secondary Structures have repetition of Φ and Ψ angles.
Also known as repetitive structures. e.g. α-helix and β Sheet.

The α-Helix

- **The structure of α-helix was deduced by Linus Pauling and Robert Corey in 1951.**
- **The right handed α-Helix is the most common unit of secondary structure.**
- **The structure of α-Helix was derived from model building of the crystallographic structure of Myoglobin.**



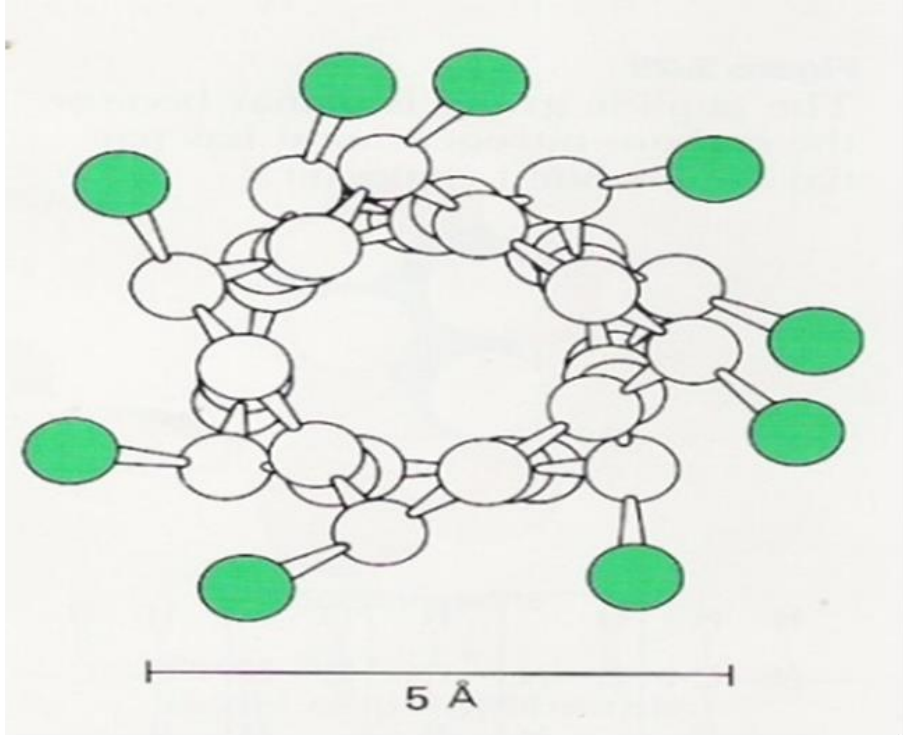
Linus Pauling and Robert Corey

A) Regular Secondary Structure

The α-Helix

- **α-Helix is a rod like structure.**

- **The tightly coiled polypeptide main chain form inner part of rod and the side chains extend outward in helical array.**



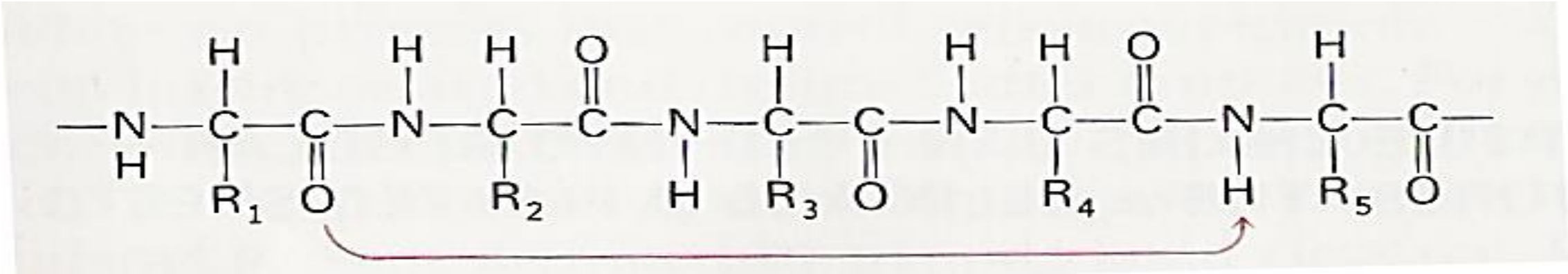
Cross-sectional view of an α-Helix. Side chains (in Green) are outside of helix in a helical array. Diameter of the helix is 5Å.

A) Regular Secondary Structure

The α-Helix

α-Helix is formed due to the hydrogen bonding between the backbone carbonyl oxygen (C=O acceptor) of one amino acid residue (*i*) and the amide hydrogen (N-H donor) of the residue four ahead (*i*+4) in the polypeptide chain.

The first four NH groups and the last four CO groups will normally lack the backbone hydrogen bonds.



In α-helix CO group of residue *i* is hydrogen bonded to NH group of residue *i*+4.

It is called 3.6_{13} helix, where 13 is the number of atoms forming the hydrogen bond between the donor (NH) and acceptor (CO) groups present in 3.6 residues. (note Hydrogen atom is included in this count).

A) Regular Secondary Structure

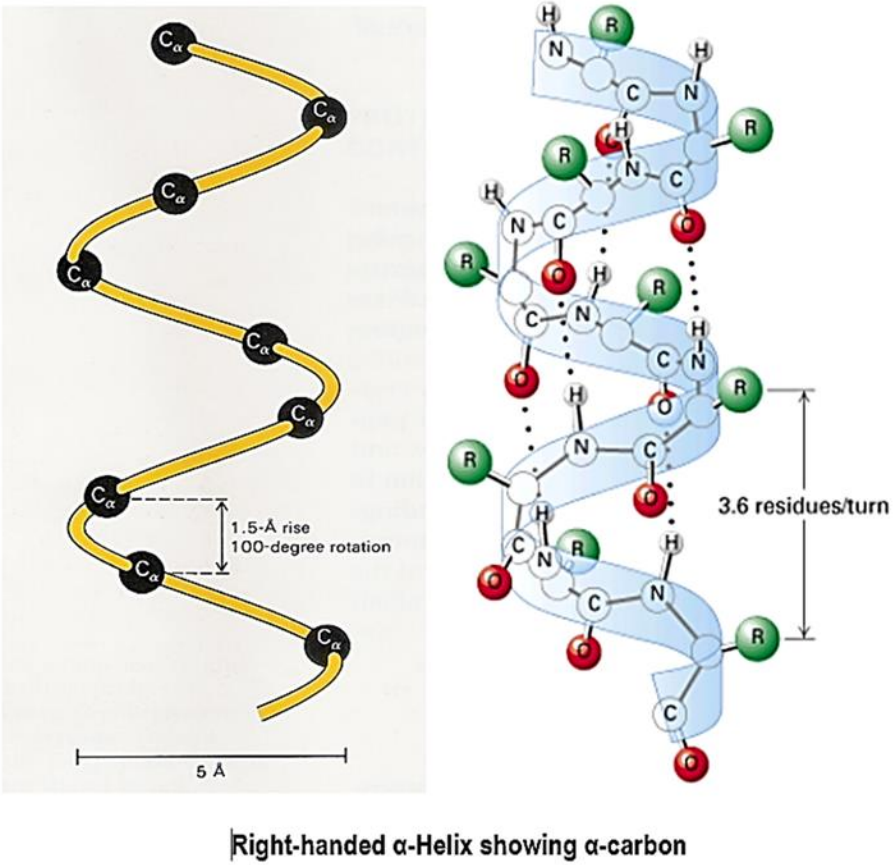
The α-Helix

Each residue is related to the next residue by a rise of 1.5 Å along the helix axis and a rotation of 100˚, hence there are 3.6 residues (360/100) per turn or in (one complete rotation).

100° is contributed by = 1 residue
360° will be = (1/100) x 360 = 3.6 residues

Translational distance (rise per residue) = 1.5 Å
Number of residue per turn = 3.6
Rise per turn (pitch) = 3.6 x 1.5 = 5.4 Å

It is called 3.6_{13} helix, where 13 is the number of atoms forming hydrogen bond between the donor (NH) and acceptor (CO) groups present in 3.6 residues. (note the hydrogen atom is included in this count).



Right-handed α-Helix showing α-carbon

A) Regular Secondary Structure (Alpha Helix)

The α-Helix

Naturally occurring α-Helix is right handed, because L-amino acids are responsible for the formation of Right handed α-Helix, while D-amino acids are responsible for the formation of left handed α-Helix. The screw sense of a helix can be right handed (clockwise) or left handed (counter clockwise).

One of the major results of model building studies was realization that the α-Helix arises from regular values for Φ and Ψ, the torsion or dihedral angle (angle between two planes). Polypeptide backbone is twisted around each α-Carbon with a (Phi) Φ -57˚ and (Psi) Ψ -47˚ angle.