

# STRUCTURE OF PROTEINS

Periodic repeats of linear Polypeptide  
Secondary structure stabilized by hydrogen bonds  
Most Common regular/ repetitive secondary structures are  $\alpha$  helix and  $\beta$  sheets

## $\alpha$ Helix

- CHARACTERISTICS**
- Right-handed helix, also called  $4_{12}$
  - Each turn has 3.6 aa residues (n) and is 5.4 Å high (pitch of)
  - Rise per residue  $(\Delta z) = p/n = 1.5 \text{ Å}$
  - Stabilized by H-bond between CO of i to NH of  $(i+4)^{\text{th}}$  aa
  - $\phi$  of  $-45^\circ$  to  $-50^\circ$   $\psi = -60^\circ$
  - Lies in lower left quadrant of R.P.
  - Peptide plane roughly parallel to helix axis
  - R-groups point outwards, and oriented towards N-terminal
  - Unfavourable amino acids in  $\alpha$ -helix: Pro, Gly, Ser, Asp, Asn, Thr, Met, Ile (Branched aa)



### Proline ( $\alpha$ -helix breaker)

- CHARACTERISTICS**
- Imino group does not have H-bond to be donated.
  - Ring structure does not allow  $100^\circ$  rotation
  - Conformational rigidity

### Glycine

- CHARACTERISTICS**
- Many allowed angles of rotation
  - Gives Conformational flexibility

## TYPES OF HELIX

- | $\alpha$ -helix                | n-helix                    | $3_{10}$ -helix            | 2 <sub>7</sub> -helix      |
|--------------------------------|----------------------------|----------------------------|----------------------------|
| $4_{12}$                       | $4.4_{10}$                 |                            |                            |
| 4 aa in a turn and             | Loosely coiled             | Tightly coiled             | 2.2 Residues per turn      |
| 13 atoms in backbone of H-bond | H-bond $i \rightarrow i+5$ | H-bond $i \rightarrow i+3$ | 7 atoms in H-bond backbone |
|                                | Rarely found               | Rarely found               | H-bond $i \rightarrow i+2$ |

## Polypyrroline Helix

- | PP-I                                                | PP-II                                                 |
|-----------------------------------------------------|-------------------------------------------------------|
| Consists of cis proline peptide bond                | Consists of trans proline peptide bond                |
| right-handed helix                                  | Left-handed helix                                     |
| $\phi, \psi, \omega = 75^\circ, 160^\circ, 0^\circ$ | $\phi, \psi, \omega = 75^\circ, 145^\circ, 180^\circ$ |

## Role of amino acids (affecting stability of $\alpha$ -helix)

- Electrostatic repulsion (or attraction) between consecutive aa residues
- Interaction between R-groups spaced 100 residues apart
- Induced dipole between aa residues at ends of helix & electric dipole inherent to helix
- Bulkiness of adjacent R-groups
- Occurrence of Pro & Gly residues

## $\beta$ -Sheet

- CHARACTERISTICS**
- Extended stretch of 5 or more aa called  $\beta$ -strand.
  - $\beta$ -strands organized next to each other to form  $\beta$ -sheets.
  - $\beta$ -strands oriented in same direction-parallel  $\beta$ -sheet.
  - $\beta$ -strands oriented in opposite direction-Antiparallel  $\beta$ -sheet.
  - H-bond pattern varies on type of sheet (straight for anti parallel, non-linear for parallel).
  - H-bond is present between adjacent peptide chains.
  - Repeating unit of  $\beta$ -sheet is 2 aa and is 7 Å in length.
  - Rise/residue: 3.47 Å - Antiparallel 3.25 Å - Parallel
  - Antiparallel  $\beta$ -sheet more stable than parallel
  - Antiparallel  $\beta$ -sheet needs hair pin turn and parallel  $\beta$ -sheets require crossover connection



## \*Beta-turn/bend

- Polypeptide chains can fold upon themselves
- Usually 4 aa to form turn
- Glycine is small and flexible: hence occurs frequently
- Proline residues found frequently and occur on protein surfaces.

## TYPES

Differ in  $\phi, \psi$  angles of 2nd and 3rd amino acid

|          | TYPE I               |                      | TYPE II              |                      |
|----------|----------------------|----------------------|----------------------|----------------------|
|          | $\phi_1 = -60^\circ$ | $\psi_1 = -30^\circ$ | $\phi_1 = -60^\circ$ | $\psi_1 = 120^\circ$ |
|          | $\phi_2 = -30^\circ$ | $\psi_2 = 90^\circ$  | $\phi_2 = 90^\circ$  | $\psi_2 = 120^\circ$ |
|          | $\phi_3 = 90^\circ$  | $\psi_3 = 0^\circ$   | $\phi_3 = -60^\circ$ | $\psi_3 = 0^\circ$   |
| I'       | $\phi_1, 60^\circ$   | $\psi_1, 30^\circ$   | $\phi_1, 90^\circ$   | $\psi_1, 0$          |
| II'      | $\phi_1, 60^\circ$   | $\psi_1, -120^\circ$ | $\phi_1, -60^\circ$  | $\psi_1, 0$          |
| IV       | $\phi_1, -61^\circ$  | $\psi_1, 50^\circ$   | $\phi_1, -53^\circ$  | $\psi_1, 17^\circ$   |
| Va & b   | $\phi_1, -60^\circ$  | $\psi_1, 120^\circ$  | $\phi_1, -90^\circ$  | $\psi_1, 0$          |
| VI a & b | $\phi_1, -135^\circ$ | $\psi_1, 135^\circ$  | $\phi_1, -135^\circ$ | $\psi_1, 160^\circ$  |
| VII      | $\phi_1, -60^\circ$  | $\psi_1, -30^\circ$  | $\phi_1, -120^\circ$ | $\psi_1, 120$        |

## Loops

- Secondary Structures are joined by additional structures called loops.

- TYPES**
- Hair pin loop**  
Often b/w antiparallel  $\beta$  strands.
  - Omega Loop**  
At beginning and end (6-38 residues)
  - $\Omega$  Loop**  
Random loop with non-repetitive  $\phi$  &  $\psi$  values
  - Extended Loop**  
More than 16 residues

## Motifs

- Small specific stable arrangement of 2<sup>nd</sup> structure
- Example: **Dehydratase**  $\beta$ - $\alpha$ - $\alpha$ - $\alpha$ -turn
- Formed to bury hydrophobic aa R-groups.
- Structural Stability achieved by excluding water (requires at least 2 layers of 2<sup>nd</sup> structure)
- Reproducible and recognizable
- Doesn't have any specific function
- Also called Super Secondary Structure

## \*Structural motifs

- Zinc Finger Motifs**  
Composed of 2 cysteine followed by 2 histidine
- Leucine Zippers**  
Leucine found every 7th position in helix & involve in hydrophobic interaction
- Transmembrane proteins**  
Also called as coiled-Coil Structure

## Domain

- Polypeptides with more than few hundred aa residues often folds into 2 or more globular units
- CHARACTERISTICS**
- Retains its 3D structure even when it is separated
  - Several motifs interact to form independent, fold and domains
  - Self folding
  - Different domains have different function

### Examples:

- $\alpha$ -helix bundle (Synzyme domain 2)
- Rossmann fold ( $\beta$ - $\alpha$ - $\beta$ ) (lactate dehydrogenase)
- Greek Key ( $\beta$ - $\beta$ - $\alpha$ - $\beta$ ) (Ig-domain)

## Quaternary Structure

- More than 1 polypeptide chain association
- Oligomeric Protein, each unit is called a sub unit.
- Subunits can be identical or different.
- Protein is either homopolymers or heteropolymers
- Oligomers are usually stabilized by disulphide bond formation.

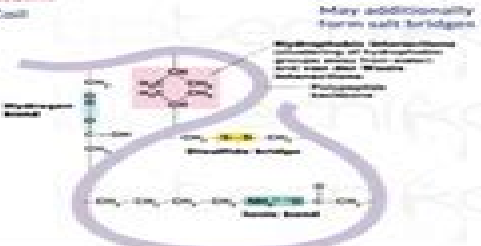


## Tertiary structure

- 3D folding or bundling up of protein
- Non-polar residues - buried inside
- Polar residues - exposed outside
- Many Proteins are organized into multiple domains

## Bonds stabilizing tertiary structure

- H-bonds
- Van der Waals interaction
- Disulphide Linkages
- Hydrophobic interaction
- Ionic interaction



# Ib Biology Notes 7 5 Proteins

**Howard E. Gendelman**



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