



**IIT Guwahati**

**Lecture 11**

**Course BT 631**

# **Protein Structure function and Crystallography**

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# Irregular secondary structures

**These are found less frequently than repetitive form, but these structures have important function.**

**In nature three types of irregular structures are found.**

- 1. Turns**
- 2. Loops**
- 3. Random Coil**

# 1. Turns

Turns connect secondary structure elements. *Turns are sharp* and show internal backbone hydrogen bond interactions and thus qualify as *bonafide* secondary structure element.

Classification of turns is based on the number of residues they contain or the **distance between residues involved in the backbone hydrogen bond interaction.**

# 1. Turns (There are 5 types of turns)

***Delta ( $\delta$ ) turn =  $i+1$*** , It is the smallest, tight turn which involves only **2 amino acid residues** and the intra-turn hydrogen bond for a delta-turn is formed between the backbone NH ( $i$ ) and the backbone CO ( $i+1$ ).

***Gamma ( $\gamma$ ) turn =  $i+2$*** , **contains 3 residues and links adjacent strands of antiparallel sheet**. The Gamma turn contains 1 residue between the H-bond. The  $\gamma$  turn is characterized by the residue in the middle of the turn  $i+1$  not participating in the hydrogen bond while first and third residue forms the H-bonds. e.g. Proteinase A, Flavodoxin and Thermolysin.

# 1. Turns (There are 5 types of turns)

**Beta ( $\beta$ ) turn =  $i+3$** , Most commonly found in protein structures and **are 4 residue turns ( $\beta$  turns) second among them is usually Proline**. Gly is often found at  $i+3$  (the  $\beta$ -turn). Here, the middle 2 residues  $i+1$  and  $i+2$  are never involved in hydrogen bonding, while  $i$  and  $i+3$  will participate in H-bonding.  $\beta$ -turn contains 2 residues between H bonds.

**Alpha ( $\alpha$ ) turn =  $i+4$** , An alpha-turn **involves 5 amino acid residues**. 3 residues are located between the Hydrogen (H) bonds.

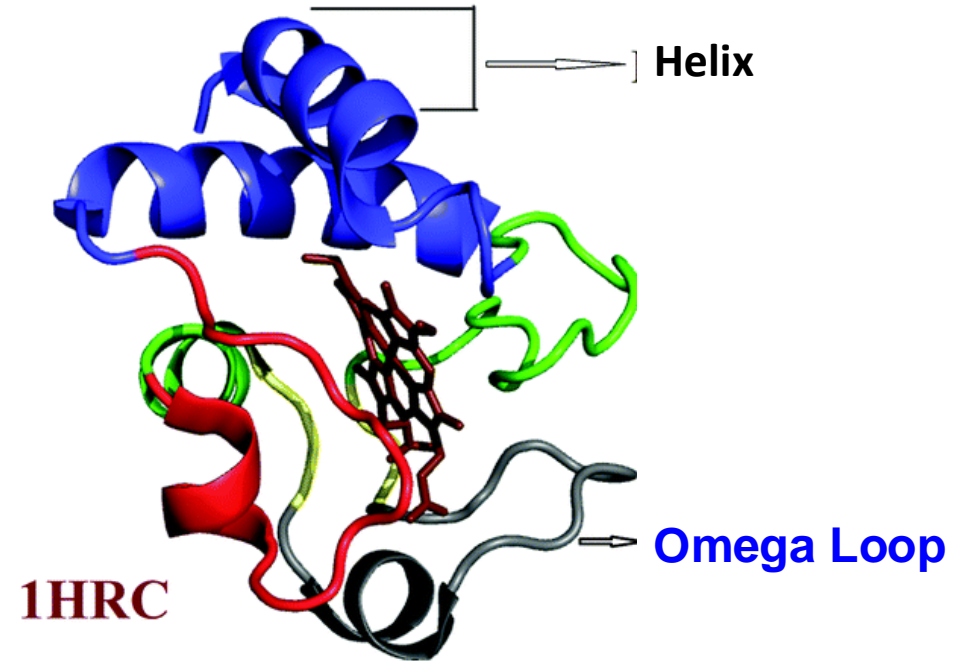
ALPHAPRED: A server for prediction of alpha turns in proteins

<http://www.imtech.res.in/raghava/alphapred/alpha.html>

**Pi ( $\pi$ ) turn =  $i+5$** , It is the largest turn which **involves 6 amino acid residues**. Contains 4 amino acid residues between the H-bonds.

## 2. Loops

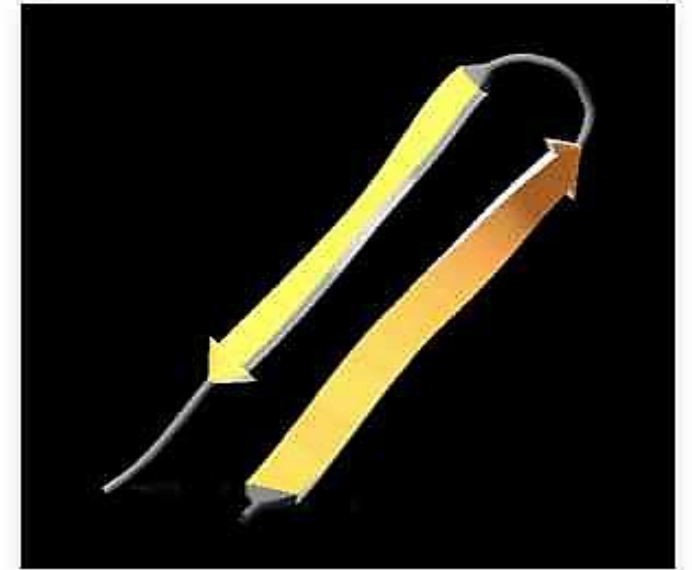
- Loops connect secondary structure elements. Loops are longer, often flexible sequences and do not belong to any class of secondary structure elements e.g. **Omega ( $\Omega$ ) loop**. It is named because of its structural resemblance with  $\Omega$ .
- **Omega loop is found in Penicillin binding protein of *E. coli* and Cytochrome C.**
- This loop consists of 6-16 amino acid residues and the distance between the two ends of loop is less than 10 Å.
- **Omega loops are involved in protein stability, folding and function.**
- They do not contain **repeating** backbone dihedral angles (but do have torsion angles) or **regular** patterns of H-bonding (but do have H-bonds).
- **Many Omega-loops contain a large number of H-bonds, therefore it is not correct to think of omega-loops as structures lacking in H-bonds.**



Cytochrome C

## 2. Loops

- The most frequent loop is  **$\beta$ -hairpin loop** connecting two antiparallel  $\beta$ -strands.
- *The two antiparallel beta strands are connected by a “hairpin” bend.*
- The presence of  $\beta$ -Hairpin provides stability to the protein structure.



(Beta hairpin loop)

What is the difference between a **Hairpin** and a **Loop**?

Hair pin consists of two  $\beta$ -strands and a small loop connects them.

## 2. Loops

### *Significance of $\beta$ -Hairpin and Omega loops*

$\beta$ -Hairpin and Omega loops are found on protein surface and they are involved in the joining of  $\alpha$ -helix and  $\beta$ -sheet.

These irregular structures are also involved in molecular recognition process.



# 3. Random Coil

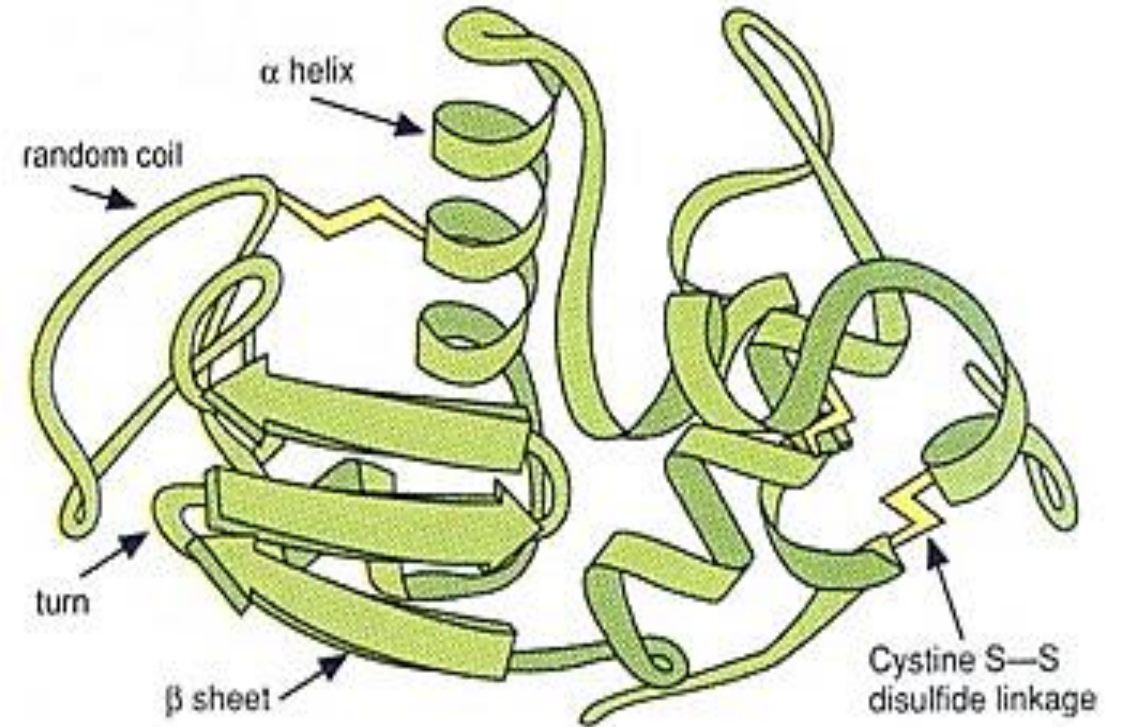
It refers to the totally disordered and rapidly fluctuating conformations assumed by denatured (fully unfolded) proteins in solution.

In native (folded) proteins, non-repetitive structures are less ordered than are  $\alpha$ -helices or  $\beta$ -sheets.

They are simply irregular and hence more difficult to describe. **Pro, Asp, Ile and Gly induce the formation of Random Coil.**

*In turns, loops and coils, the residues must still have allowable backbone torsion angles.*

*It is a grave mistake to believe that a polypeptide in random coil conformation can have random  $\Phi$  and  $\Psi$  torsion angles.*



(Secondary structure showing  $\alpha$ -helix,  $\beta$ -strand and the turn and random coil)