



IIT Guwahati

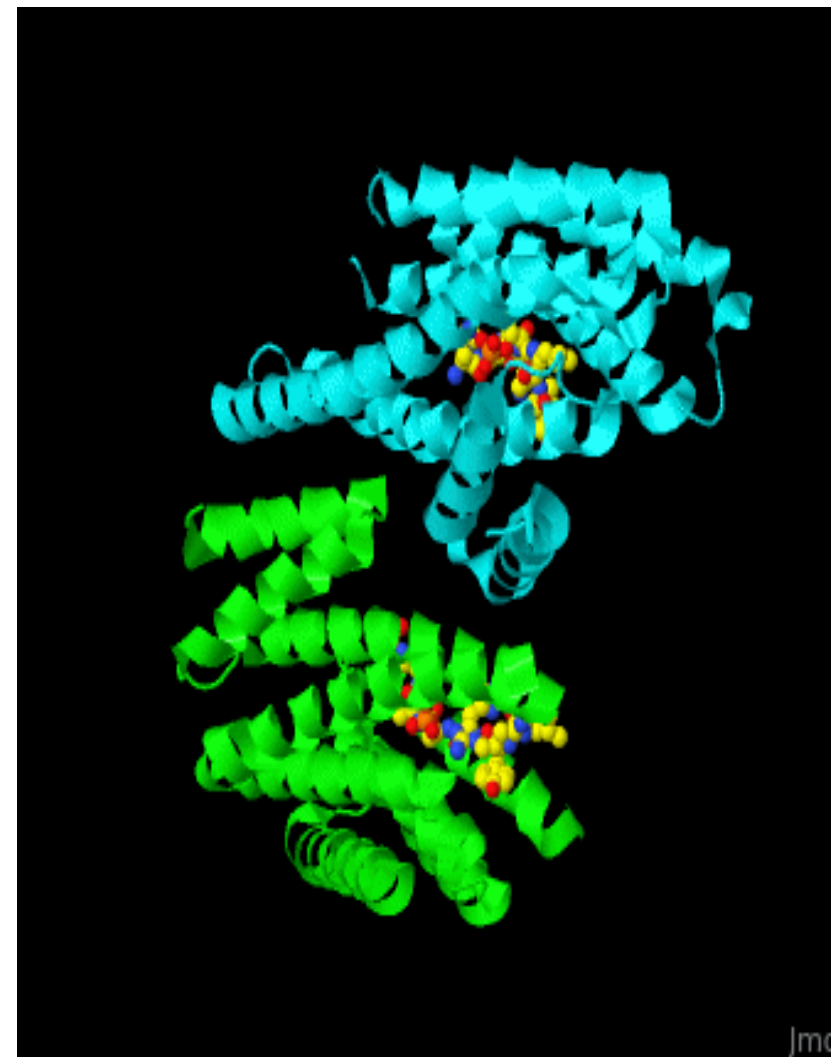
Lecture 10

Course BT 631

Protein Structure function and Crystallography

Prof. Arun Goyal

Dept. of Biosciences and Bioengineering



Secondary Structure

The β -Strand based Sheet structure

- β -Strand is so called because it was the second unit of secondary structure predicted from model building by Pauling and Corey in 1951. They discovered another periodic structural motif, which they named as β -strand.
- Despite its name, the β -strand is a helical arrangement although an extremely elongated form, with 2 residues per turn and translational distance of 3.4 Å. This leads to a pitch (repeat distance) of 6.8 Å in a regular β -strand.
- When two or more β -strands form additional hydrogen bonding interactions a stable sheet like arrangement is created. These β -sheets (or β -pleated sheets) result in significant overall stability and are stabilized by formation of backbone hydrogen bonds between adjacent strands.

Secondary Structure

The β -Strand based Sheet structure

β -pleated Sheet Stabilizers: Met, Val, Ile and Cys.

β -pleated Sheet de-stabilizers: Glu, Pro, Asn, His.

β -pleated Sheet has Φ angle (-119 to -139) and
 Ψ angle (+113 to +135)

Chymotrypsin contains predominantly β -strands.

Secondary Structure

The β -Sheet vs α -helix

- β -Sheet is markedly different from the α -helix in that it is a sheet rather than a rod. A polypeptide chain in the *β -pleated sheet* is almost fully extended rather than being tightly coiled as in the *α -helix*.
- The axial distance between adjacent amino acid is 3.4 Å. in contrast with 1.5 Å for the α -helix.
- Another difference is that the β -pleated sheet is stabilized by hydrogen bonds between NH and CO groups in different polypeptide chain, whereas in the α -helix the hydrogen bonds are between NH and CO groups in the same polypeptide chain.

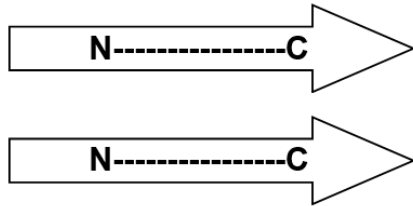
There are two major classes of beta-sheets:

A) the parallel beta-sheet

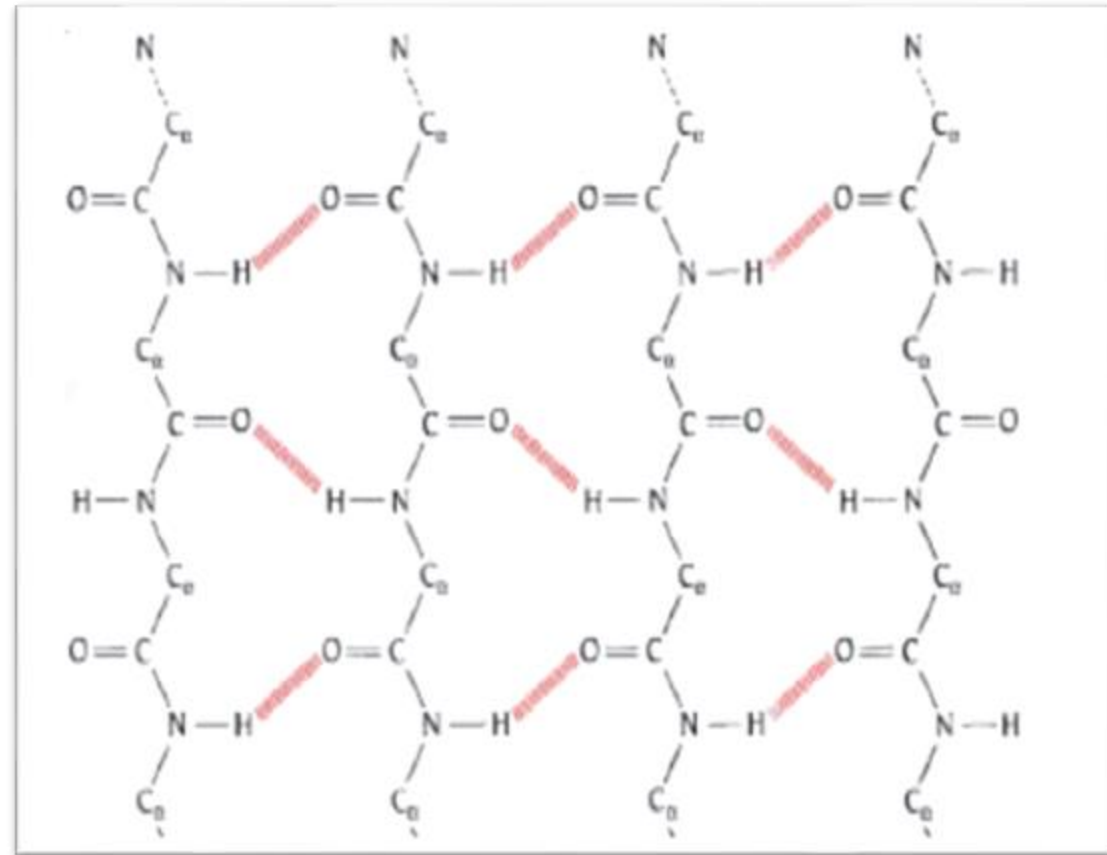
B) the antiparallel beta-sheet

The *Parallel* β -Sheet

- The *Parallel* β -Sheet is characterized by two polypeptide strands running in the same direction held together by hydrogen bonds.



- The strands in figure represent parallel β -sheet with **N-Terminals at Top** and **C-terminals at Bottom**.
- The **red** lines represent hydrogen bonds between the strands.
- Without seeing the ends of the peptide it can be difficult to tell which direction a peptide strand is running.

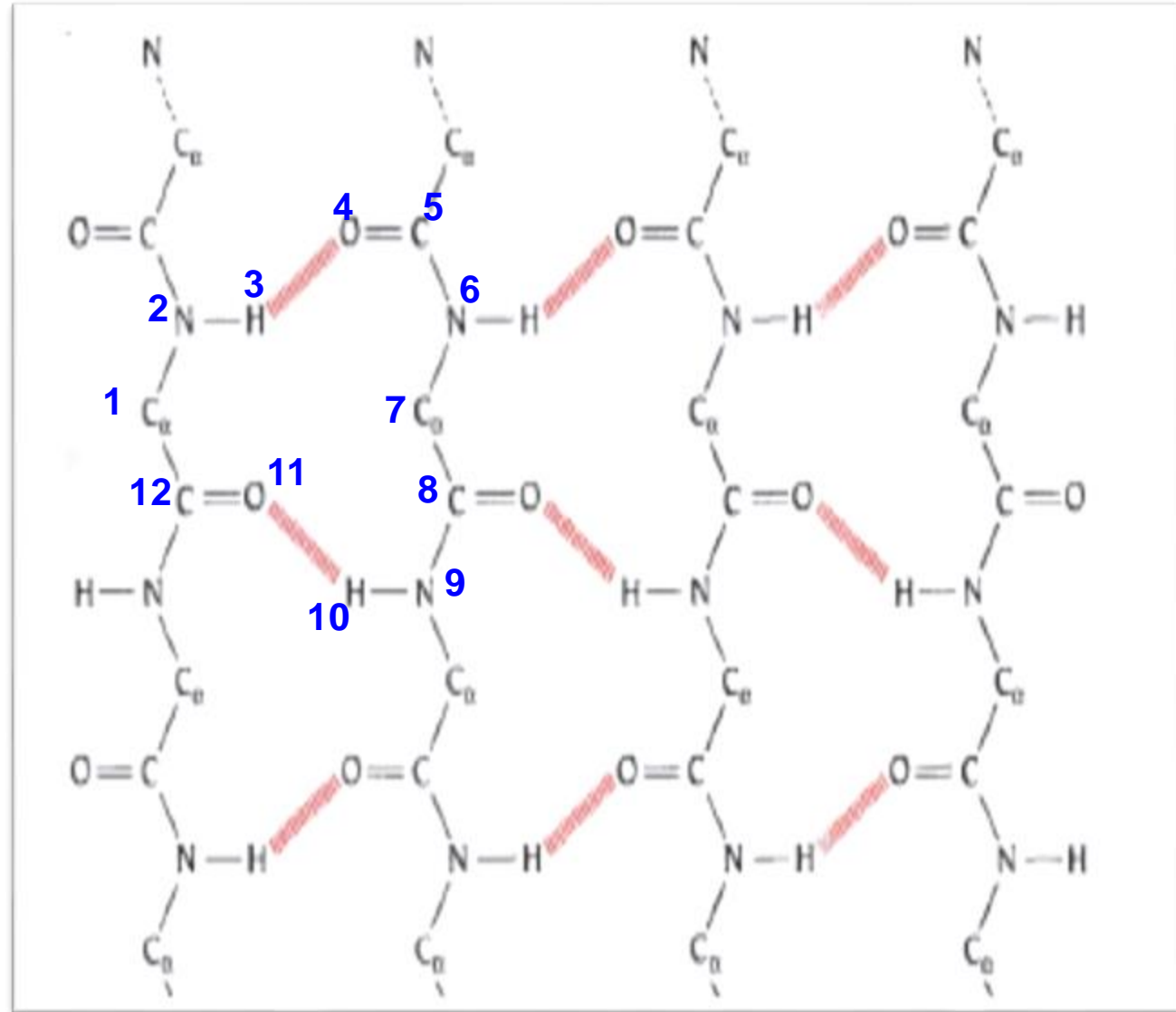


The *Parallel* β -Sheet

How then does one tell, if two adjacent strands are running in the same direction or opposite directions?

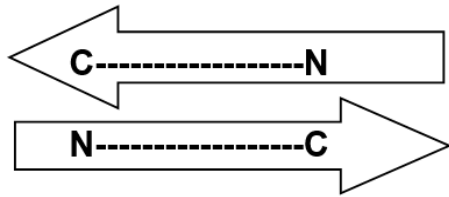
That is done by counting the number of atoms in the hydrogen bonded rings.

In parallel β -sheets each hydrogen bonded ring has 12 atoms in it.

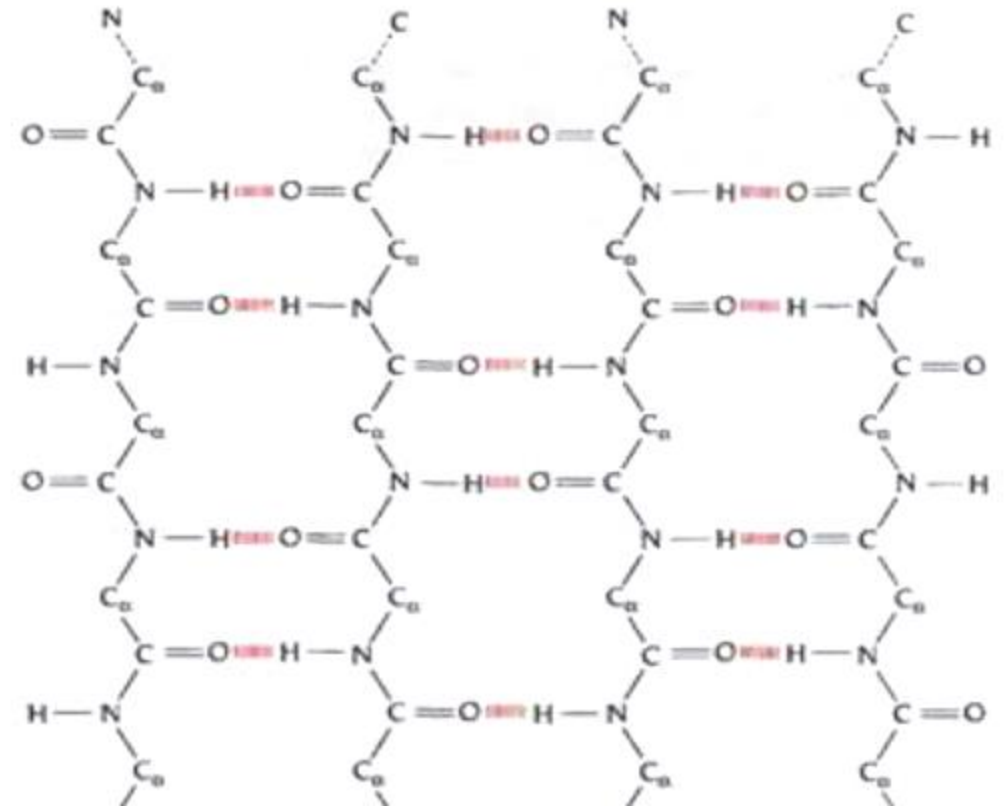


The *Anti-parallel* β -Sheet

- The *Anti-parallel* β -Sheet is characterized by two polypeptide strands running in opposite directions held together by hydrogen bonding between the strands.

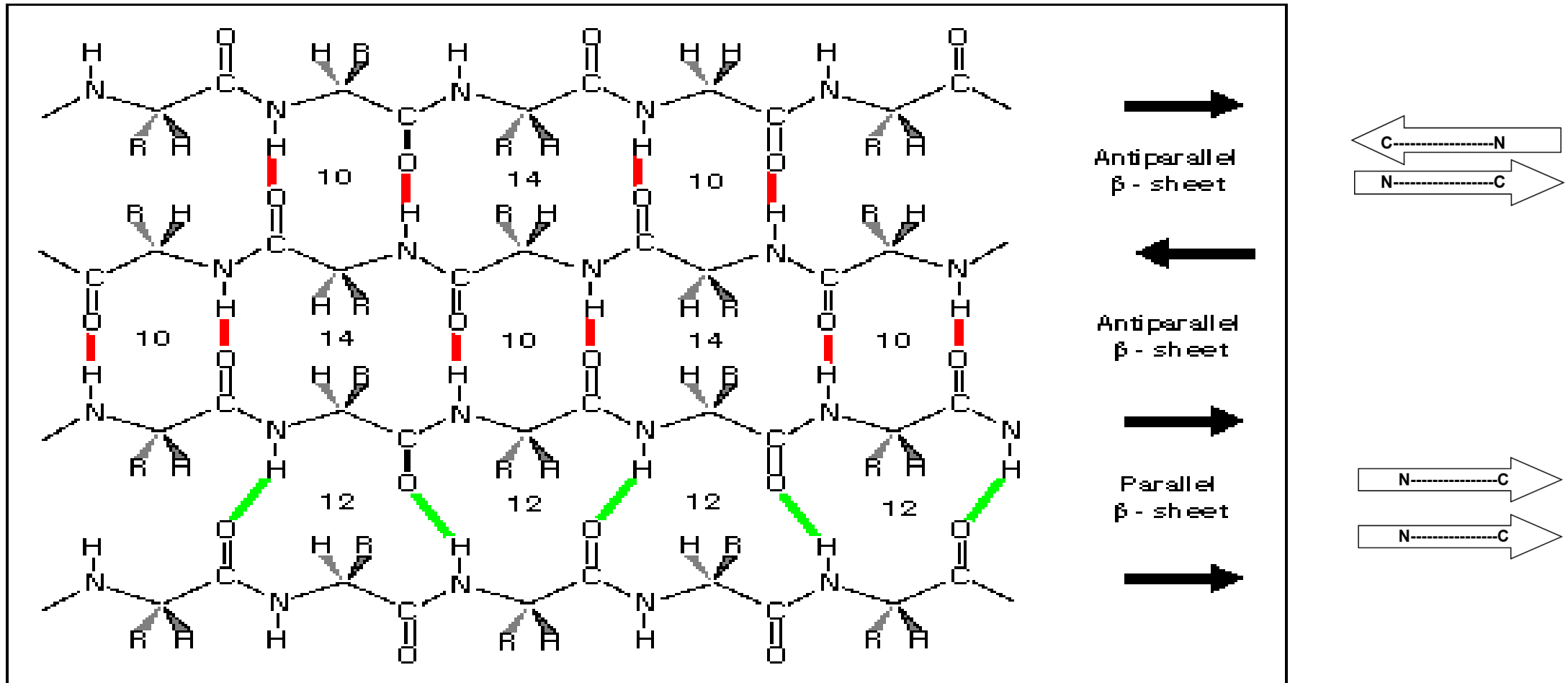


- The strands in figure represent antiparallel β -sheets with **N-Terminals and C-terminals in opposite directions**.
- The **red lines** are hydrogen bonds between the strands.
- One can recognize an antiparallel β -sheet by the number of atoms in the hydrogen bonded rings.
- The number of atoms in hydrogen bonded rings **alternate between 14 and 10** in an anti-parallel β -sheet.
- The Hydrogen bonds in an antiparallel β -sheet are linear. For this reason the antiparallel β -sheets are more stable than parallel β -sheets.



(anti-parallel is dominant over parallel structure).

The top three strands show **Antiparallel β -sheets**. H-Bond in **Red** (Number of atoms 14 and 10)



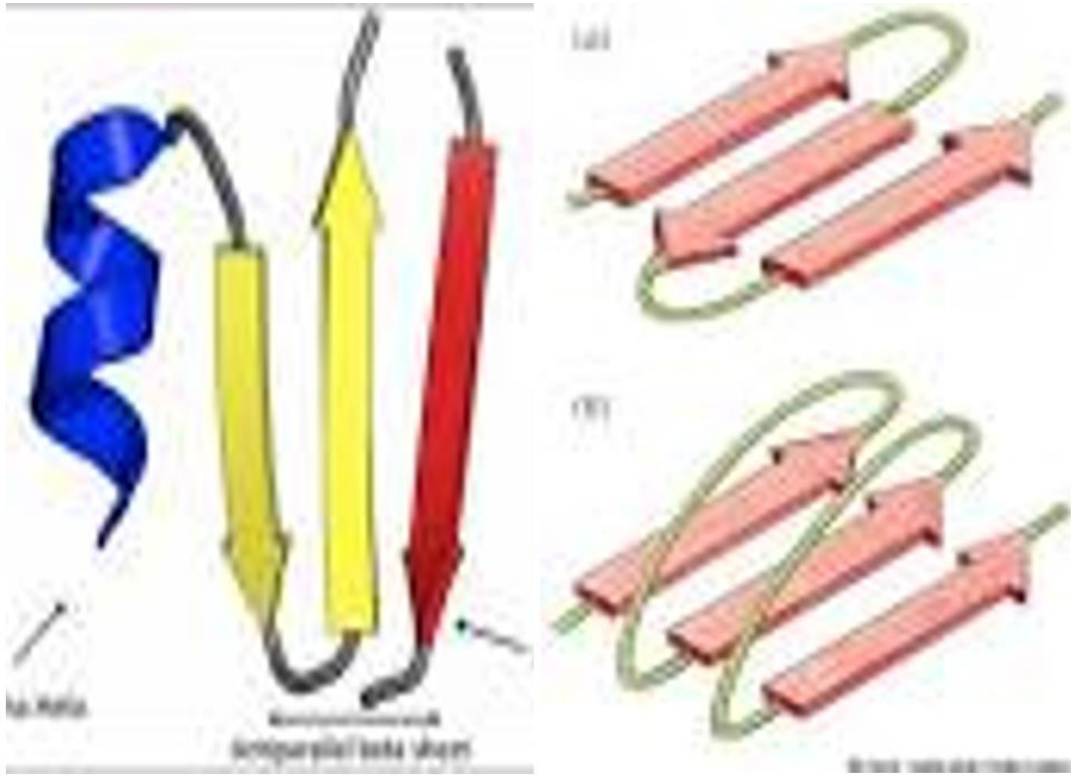
Bottom two strands show **Parallel β -sheets**. H-bond in **Green**. H-bonded ring has 12 atoms

Torsion angle and number of residues per turn for regular Secondary Structures

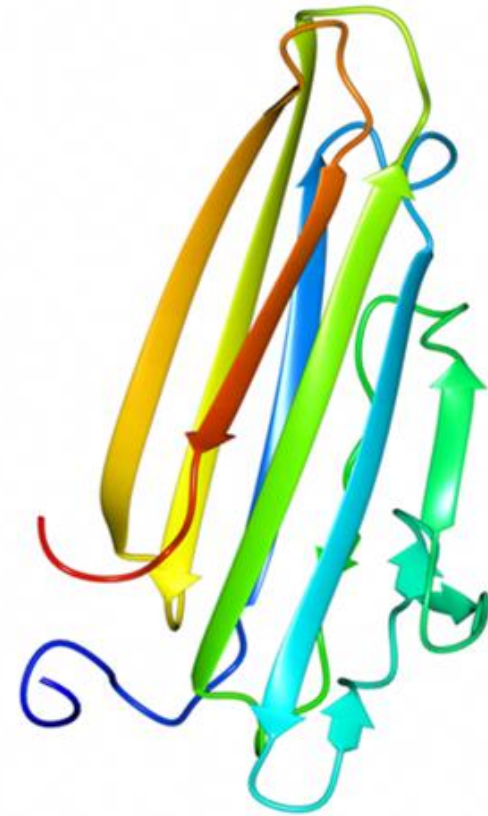
Table: Torsion angle, translation distance and number of residues per turn for regular secondary structure.

Secondary structure element	Torsion angle (°)		Residue/turn	Translational distance per residue (Å)	Pitch (Å)	No. of atoms, Shape
	ϕ	ψ				
Right-handed α - Helix	- 57	- 47	3.6	1.5	5.4	13, Normal
3_{10} Helix	- 49	- 26	3.0	2.0	6.0	10, Tight
π -helix	- 57	- 70	4.4	1.15	5.06	16, Loose
Parallel β Pleated Sheet	-119	+113	2.0	3.2	6.4	Elongated
Anti-parallel β Pleated Sheet	-139	+135	2.0	3.4	6.8	Elongated
Left-handed α - Helix	+57	+47	-	-	-	-

Beta-sheets



(Anti-parallel and Parallel β -strands)

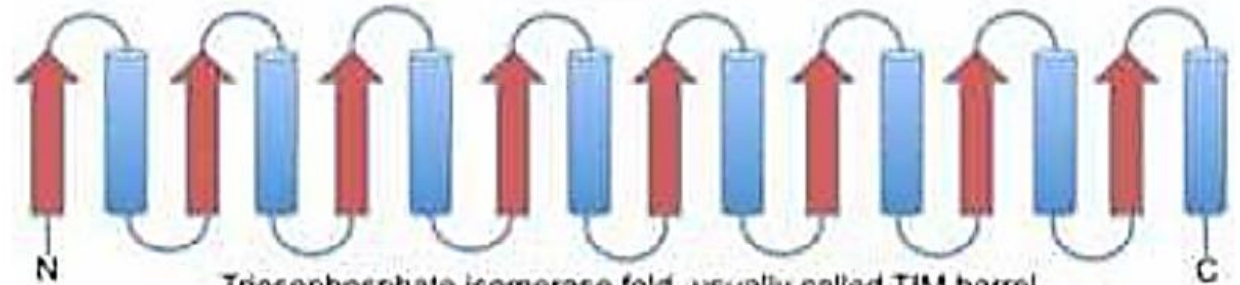


(β -Sandwich)
Antiparallel β -sheet

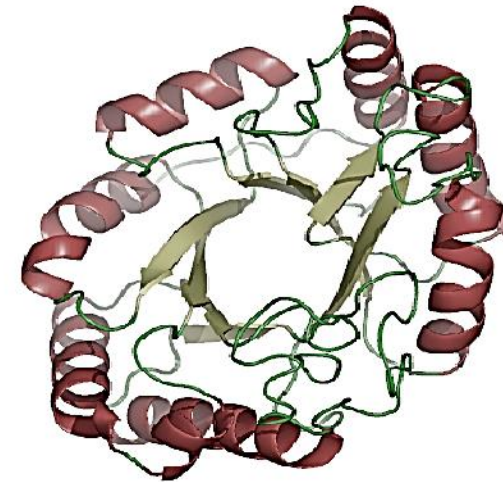
Beta-sheets



(β -Barrel) Anti-parallel sheets rolled into cylinder
Outer membrane of Gram-negative bacteria, Porins



Triosephosphate isomerase fold, usually called TIM barrel fold, is very often found in proteins with no direct functional relationships



Lichenase displays a TIM Barrel, (β/α) 8-fold, common in glycoside hydrolase families.