Course BT 631

Protein Structure function and Crystallography

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A) Regular Secondary Structure (Alpha Helix)

The α-Helix

Hydrogen bonds are 2.86 Å long, linear and lie (in a regular helix) in parallel to the helical axis. Hydrogen bond has directionality due to the electronegative oxygen atom. Similarly, peptide bond also has polarity and the combined effect of these two parameters give α-helices pronounced dipole moments.

The amino end (N-Terminal) of α-Helix has positive charge and carboxyl end (C-Terminal) has negative charge.

Glutamic Acid, Alanine, Leucine, Histidine are Helix Stabilizer amino acid residues, whereas

Glycine, Proline, the Helix destabilizer amino acid residues.

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- **Proline residues induce distortions of around 20° in the direction of the helix axis. This is because proline cannot form a regular alpha-helix due to steric hindrance arising from its cyclic side chain which also blocks the main chain N atom and chemically prevents it forming a hydrogen bond.**
- **Proline does not form helical structure as the amide proton of N-H prevents the hydrogen bonding and the side chain covalently bonded to the N atom restricts the backbone rotation. The result is that the proline is often located at the beginning of helices or in the turns between 2 helical units.**
- **Proline distorts the helix causing a kink or changes the direction of polypeptide chain.**

A) Regular Secondary Structure (Alpha Helix)

The α-Helix

- **The α-helix content of proteins is highly variable.**
- **The α-helix is the major structural motif in myoglobin and hemoglobin and they contain 80% and 75% α-helix, respectively.**
- **Other protein such as chymotrypsin, is virtually devoid of α-helix.**
- **In most proteins the single stranded α-helix is usually short rod and less than 40 Å in length.**
- **The α-helical is extended in some proteins to much longer rod, as long as 1000 Å (100 nm or 0.1 μm) or more.**
- **Two or more such α-helices can form a cable. Such α-coiled coils are found in keratin in hair, myosin and tropomyosin in muscle, epidermin in skin and fibrin in blood clots.**

A) Regular Secondary Structure

Other helical conformations (The 3_{10} helix)

The 3_{10} helix

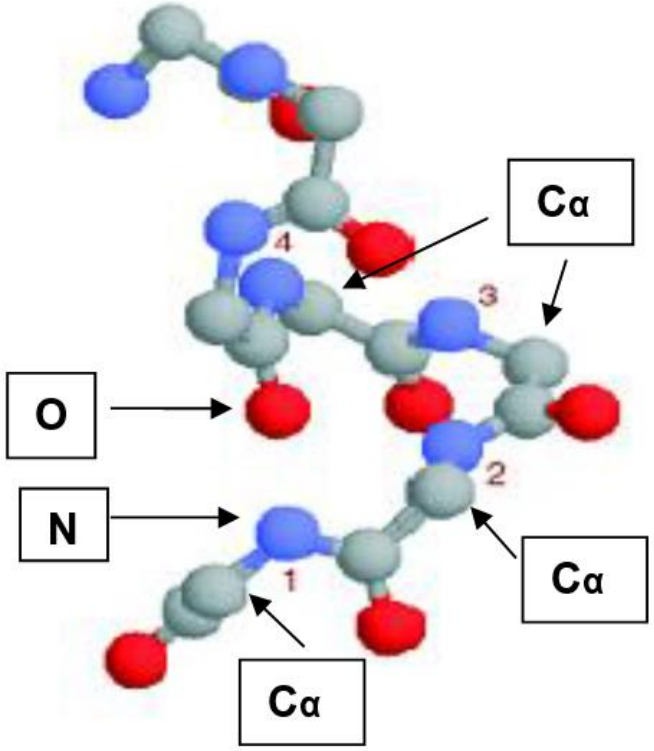
The 3_{10} helix is a structural variation of the α-helix found in proteins.

It is found when a regular α-helix is distorted by the presence of unfavorable residues, near a turn region or when short sequences fold into helical conformation.

In the 3_{10} helix the hydrogen bonds are formed between residues (*i* and *i*+3) in contrast to residues (*i* and *i*+4) in regular α-helix.

The name 3_{10} arises because there are 3 residues per turn and 10 atoms enclosed in a ring formed by each hydrogen bond (note the hydrogen atom is included in this count).

With 3 residues per turn, 3_{10} helix is tighter and narrower.



In 3_{10} helix the hydrogen bonds are formed between residues (*i*, *i*+3)

A) Regular Secondary Structure

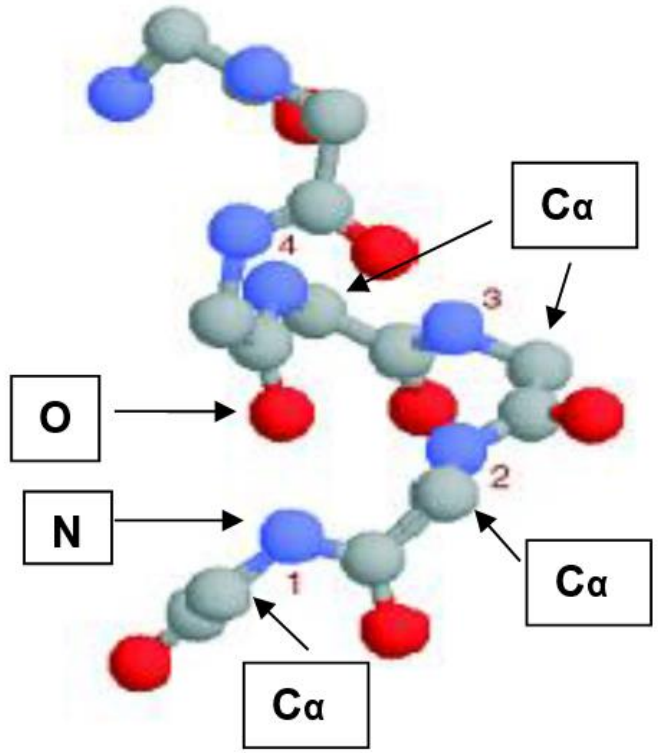
Other helical conformations (The 3_{10} helix)

The 3_{10} helix

The torsion angles are: Φ= -49 and Ψ= -26.

The rise per residue is 2.0Å.

The 3_{10} helices do occur, but are not very long, they are sometimes found at the end of α-helix.



In 3_{10} helix the hydrogen bonds are formed between residues (*i*, *i*+3)

A) Regular Secondary Structure

Other helical conformations (The π-helix)

The π-helix

A third possibility is a more loosely coiled helix with hydrogen bonds formed between the C=O and N-H groups separated by five residues (*i* and *i*+5).

This structure is the π-helix found in soybean lipoxygenase.

There are 4.4 residues per turn and 16 back bone atoms in the H-bond.

The torsion angles are: Φ= -57 and Ψ= -70.

The π-helix is more compact, more compressed than the α-helix.

The H-bonds in the π-helix are not straight and side chains interfere.

The π-helix has the larger radius of the π-helix means that backbone atoms do not make vander Waals contact across the helix axis.

A) Regular Secondary Structure

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	-	-	-	-