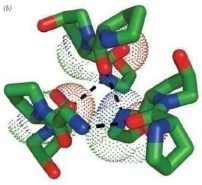
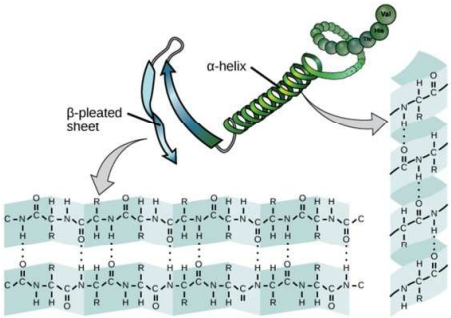


Secondary Structure

- Defined as the local conformation of protein backbone
- Primary Structure —folding— Secondary Structure
- α helix and β sheet

Secondary Structure

Regular Secondary Structure (α-helices, β-sheets)

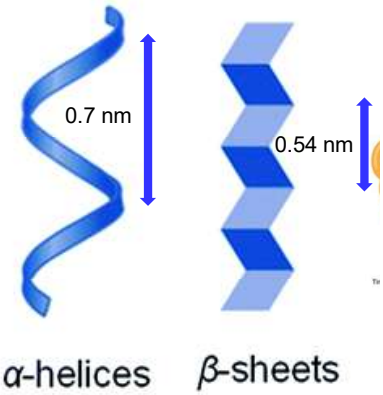


Irregular Secondary Structure (Tight turns, Random coils, bulges)

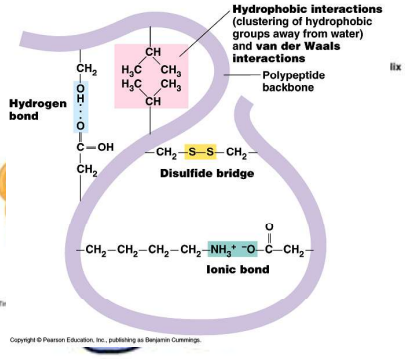
https://www.khanacademy.org/science/biology/macromolecules/proteins-and-amino-acids/a/orders-of-protein-structure

Primary structure

Secondary structure



Tertiary structure

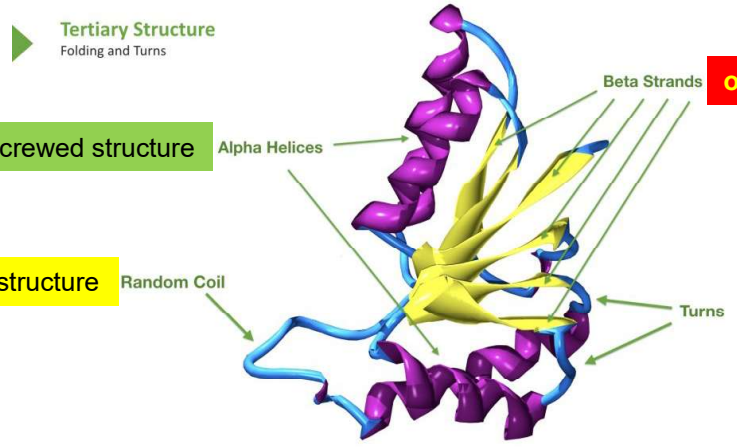


Quaternary structure

eets

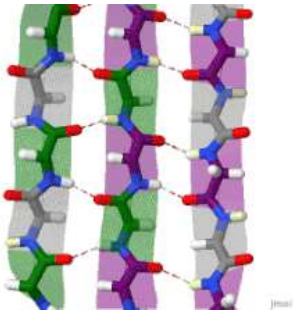
ices

https://www.toppr.com/en-ar/content/concept/advanced-knowledge-of-structure-of-protein-200359/

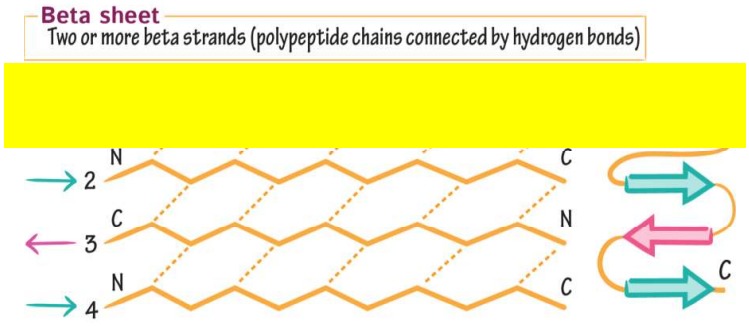


β-Sheet: A β-sheet is a common secondary structure in proteins, formed by linking two or more β-strands side by side through hydrogen bonds. The β-strands in a β-sheet can be either parallel (running in the same direction) or antiparallel (running in opposite directions). β-sheets are often depicted as flat arrows pointing in the direction of the polypeptide chain. They provide structural stability and are often found in the core of proteins.

β-Strand: A β-strand is a single stretch of polypeptide chain that is almost fully extended. It typically consists of 5-10 amino acids. In a protein, multiple β-strands come together to form a β-sheet through hydrogen bonding between the backbone atoms of the strands. While β-strands themselves are not stable structures, their stability comes from the formation of β-sheets.



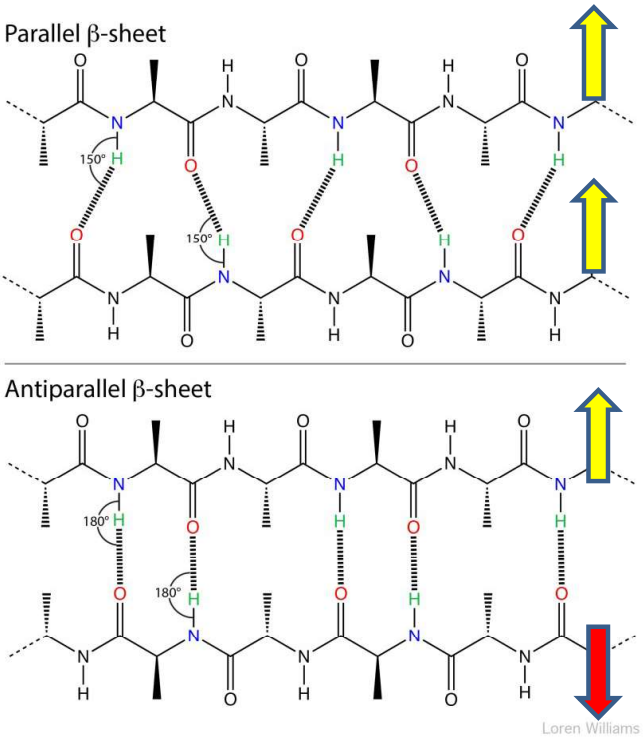
https://en.wikipedia.org/wiki/Beta_sheet



https://ditki.com/course/biochemistry/glossary/biochemical-pathway/beta-sheets-aka-beta-pleated-sheets

β-sheets

The hydrogen bonds in antiparallel β-sheets are linear, while the hydrogen bonds in **parallel** β-sheets are non-linear.



β-strand

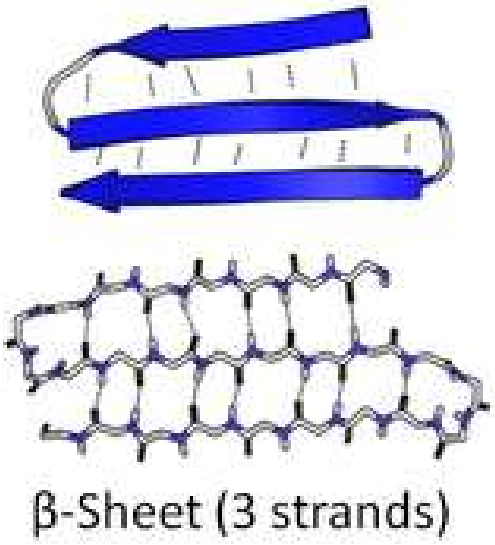
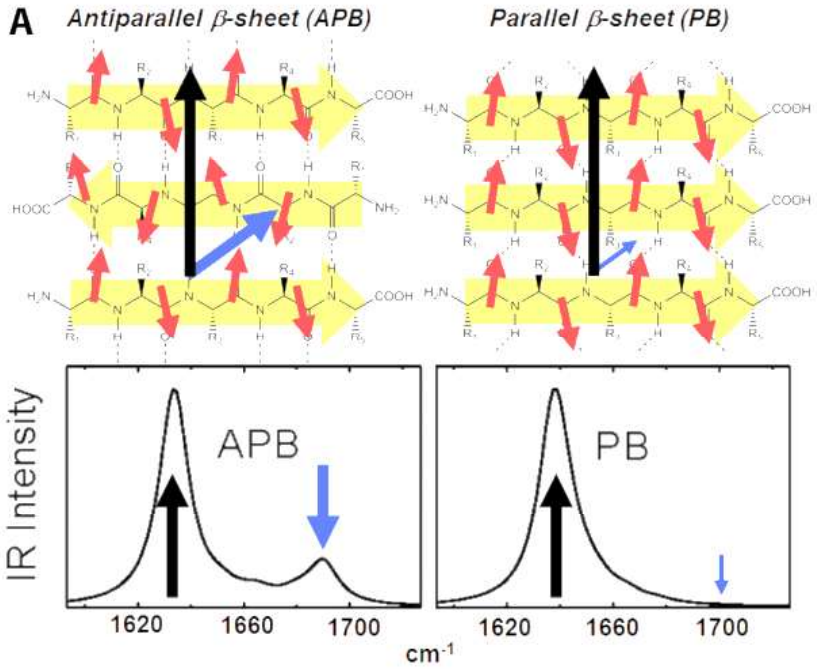


Figure illustrates the **non-linearity of parallel β-sheet hydrogen bonds** and the **linearity of antiparallel β-sheet hydrogen bonds**.

https://www.x-mol.com/groups/Dong/news/1653

Vibrational Coupling in β-Sheets Determines Amide I Spectral Features



Vibrational coupling between transition dipole moments causes excitonic delocalization within β-sheets, producing collective normal modes. In IR spectra, β-sheets show a strong low-frequency mode common to both parallel and antiparallel structures, while the high-frequency mode differs in strength and position, being more prominent in antiparallel β-sheets.

Recommended Conservative Assignment

Wavenumber region	Recommended assignment
1610–1640 cm^{-1}	β-sheet / aggregated β-sheet
1640–1650 cm^{-1}	Random coil / unordered structure
1650–1660 cm^{-1}	α-helix
1660–1680 cm^{-1}	β-turn / turns
1680–1700 cm^{-1}	β-turns and/or the high-frequency component of antiparallel β-sheet

References

1) 1,692 cm$_{-1}$ (β-turns, or the high-frequency component of anti-parallel β-sheets)
2) 1,678 cm^{-1} (parallel β-sheets)
3) 1,661 cm^{-1} (α-helix)
4) **1,645 cm^{-1} (random coils)**
5) **1,630 cm^{-1} (β-sheet / aggregated β-sheet low-frequency component)**
6) 1,610 cm^{-1} (aromatic rings)

e-PS, 6, 129(2009)

nature protocols,10, 3, 385(2015)

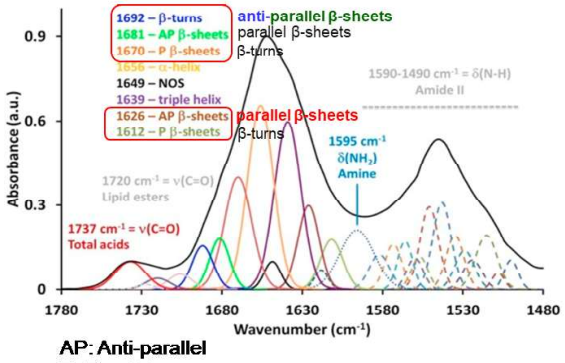
TABLE 1 | Deconvoluted amide I band frequencies and assignments to secondary structure for protein in D_2O and H_2O media.

H_2O[a]		D_2O[b]	
Mean frequencies	Assignment	Mean frequencies	Assignment
1,624 ± 1.0	β-sheet	1,624 ± 4.0	β-sheet
1,627 ± 2.0	β-sheet	1,631 ± 3.0	β-sheet
1,633 ± 2.0	β-sheet	1,637 ± 3.0	β-sheet
1,638 ± 2.0	β-sheet	1,641 ± 2.0	3_{10}-helix
1,642 ± 1.0	β-sheet	1,645 ± 4.0	Random
1,648 ± 2.0	Random	1,653 ± 4.0	α-helix
1,656 ± 2.0	α-helix	1,663 ± 4.0	β-turn
1,663 ± 3.0	3_{10}-helix	1,671 ± 3.0	β-turn
1,667 ± 1.0	β-turn	1,675 ± 5.0	β-sheet
1,675 ± 1.0	β-turn	1,683 ± 2.0	β-turn
1,680 ± 2.0	β-turn	1,689 ± 2.0	β-turn
1,685 ± 2.0	β-turn	1,694 ± 2.0	β-turn
1,691 ± 2.0	β-sheet		
1,696 ± 2.0	β-sheet		

[a]Data are from Dong and colleagues[5,47,48,54].
[b]Data are from Susi and colleagues[4,5,13,46].

1) 1,690 cm^{-1} (β-turns and/or high-frequency component of antiparallel β-sheet),
2) 1,680 cm^{-1} (β-turns and/or possible antiparallel β-sheet component),
3) 1,668 cm^{-1} (β-turns),
4) 1,658 cm^{-1} (α-helix),
5) **1,647 cm^{-1} (unordered),**
6) 1,638 cm^{-1} (triple helix),
7) **1,625 cm^{-1} (β-sheet / aggregated β-sheet low-frequency component),**
8) 1,612 cm^{-1} (aggregated β-sheet / strongly hydrogen-bonded β-sheet).

Anal Bioanal. Chem., 386,1961 (2006)



AP: Anti-parallel
P: Parallel

Trends in Analytical Chemistry, 82, 443(2016)

1) 1,715 cm^{-1}, esters,
2) **1,690 cm^{-1}, (β-turns and/or high-frequency component of antiparallel β-sheet),**
3) 1,679 cm^{-1}, parallel β-strand (in a β-sheet structure),
4) **1,668 cm^{-1}, β-turn,**
5) 1,656 cm^{-1}, α-helix,
6) **1,647 cm^{-1}, unordered structure,**
7) 1,638 cm^{-1}, triple helix,
8) **1,628 cm^{-1}, (β-sheet / aggregated β-sheet low-frequency component),**
9) **1,617 cm^{-1}, (aggregated β-sheet / strongly hydrogen-bonded β-sheet),**
10) 1,592 cm^{-1}, amine, (N–H),

TRENDS in Biotechnology, 24 ,10(2006)