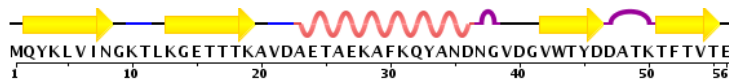


Protein Structure

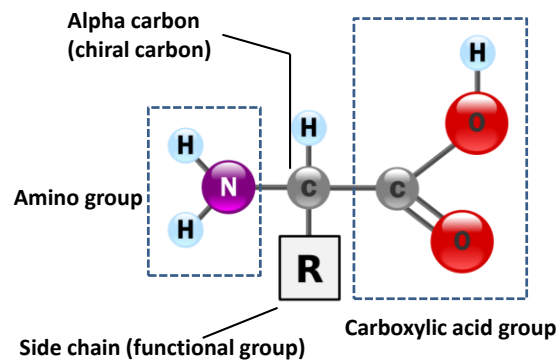
Biochemistry Boot Camp 2018
Session #1
Dinusha Jinasena
dsj125@msstate.edu

Different representations of proteins



Cartoon Model

• Amino Acids

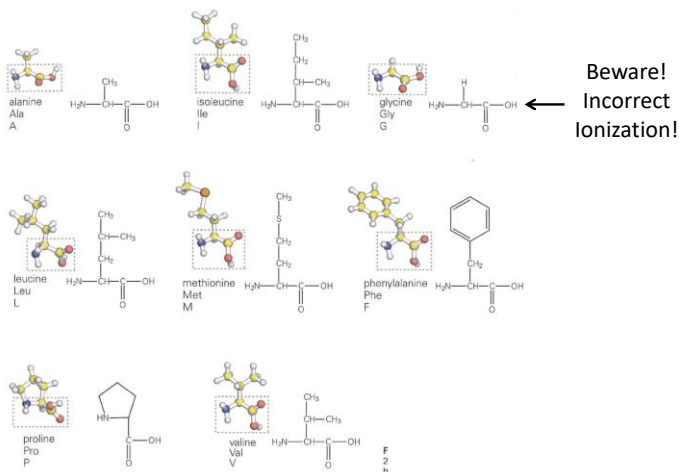


PDB code:2OED

Nonpolar Amino Acids

(side chain is uncharged at neutral pH, cannot participate in hydrogen bonding)

nonpolar, hydrophobic residues



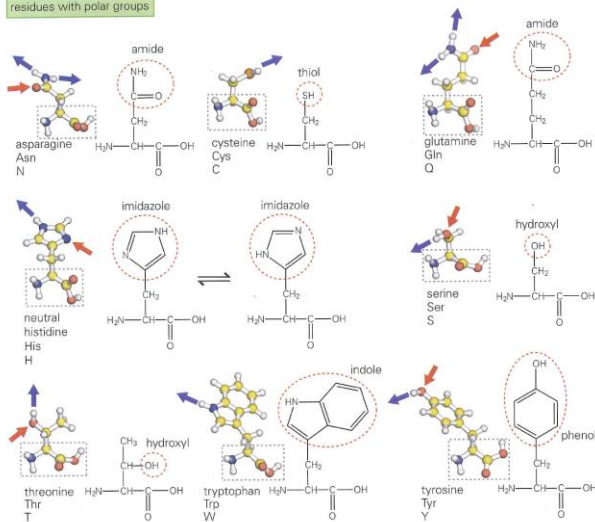
Molecules of Life, pp. 26-7

3

Polar Amino Acids

(side chain is uncharged at neutral pH, can donate or accept hydrogen bonds)

residues with polar groups



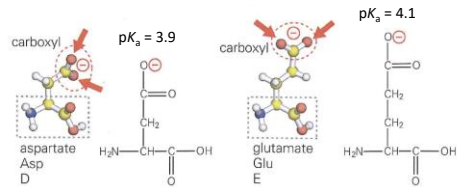
Molecules of Life, pp. 26-7

4

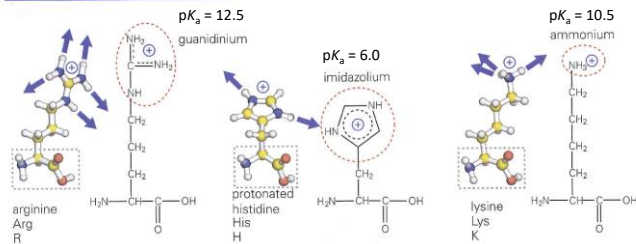
Ionizable Amino Acids

(with typical side-chain pK_a values, charged at neutral pH)

negatively charged, hydrophilic residues



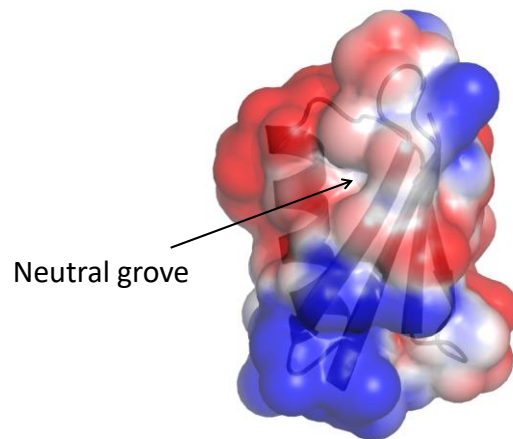
positively charged, hydrophilic residues



Molecules of Life, pp. 26-7

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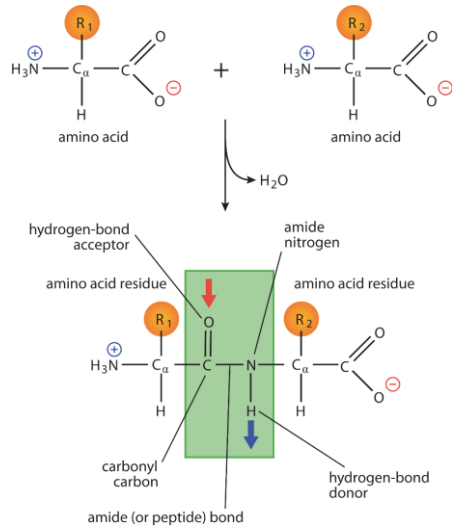
Electrostatic surface



Red – negative charge

Blue – positive charge

Making Peptide Bonds: Condensation



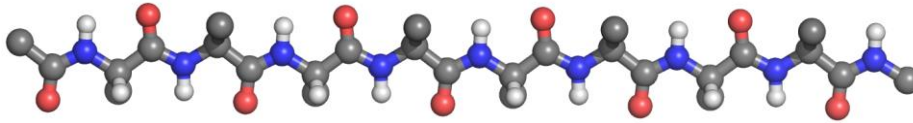
Molecules of Life, pp. 28

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Think and Discuss

What's the advantage to having twenty amino acids?

The Protein “Backbone”

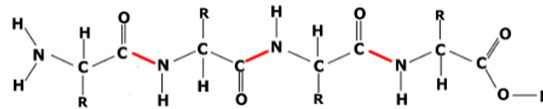


Blue: N

Grey: C_α, C_{COOH}

Red: O

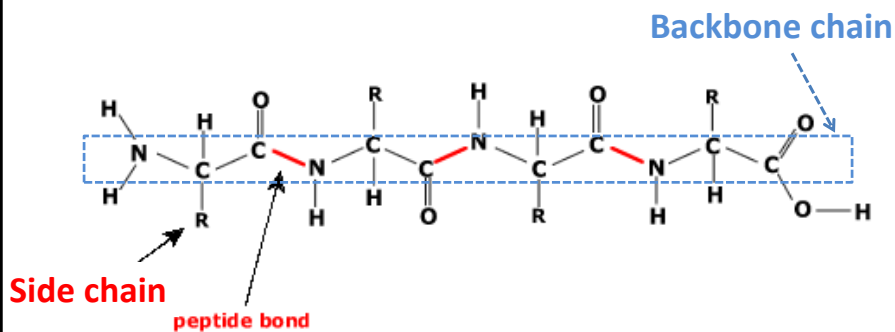
White: H_α, H_{NH}



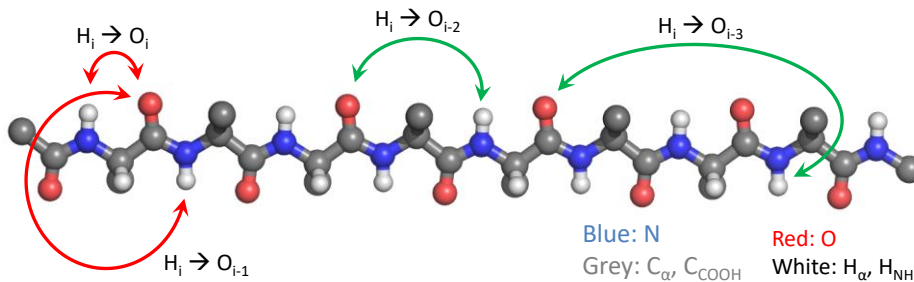
- Directionality: NT → CT is convention
- Atom names describe position in chain
- Side chains are added to the backbone

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The Protein “Backbone”



Backbone Hydrogen Bonding

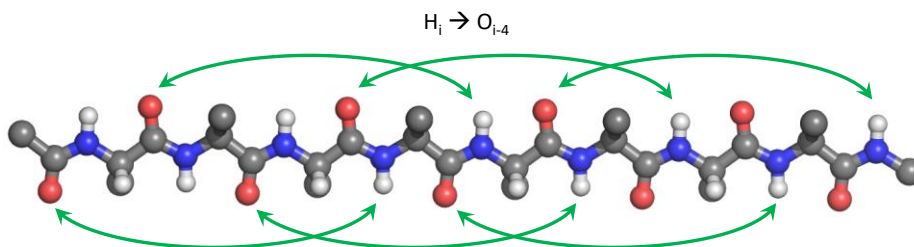


- Non-repeating backbone patterns:
 - **Too much strain:** $H_i \rightarrow O_i$ and $H_i \rightarrow O_{i\pm 1}$ hydrogen bonds
 - **Rare, but possible:** $H_i \rightarrow O_{i-2}$ (Gamma turns)
 - **Frequently observed:** $H_i \rightarrow O_{i-3}$ (Beta turns)

H-bond: H-O, N, F

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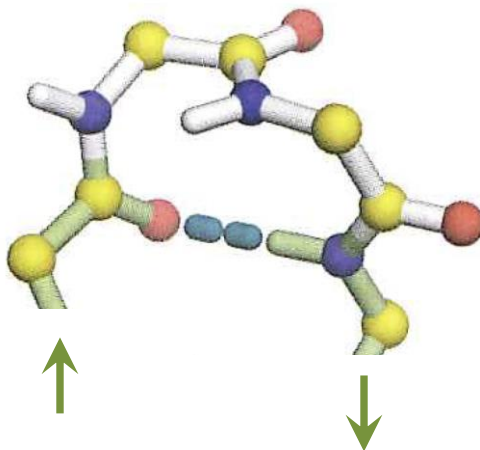
Backbone Hydrogen Bonding



- The Alpha Helix Can be Repeated
 - $H_i \rightarrow O_{i-4}$ (Gamma turns)
 - Average ϕ is -60° , Average ψ is -40°

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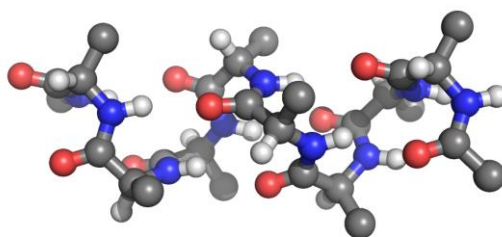
Beta Turns Reverse the Direction of the Backbone



Molecules of Life, pp. 147

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A (Right-Handed) Alpha Helix

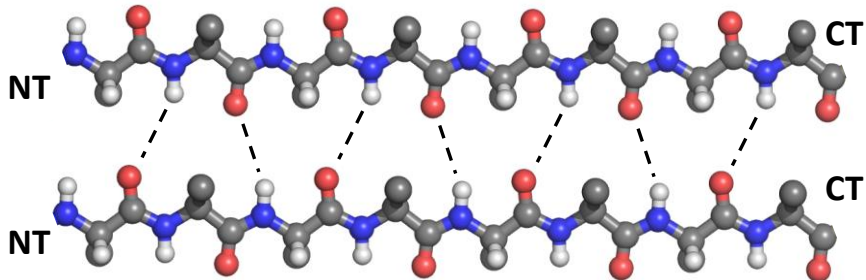


- Download helix.pdb from the course website for a model you can examine in PyMOL
- Notice that helix ends have unsatisfied H-bonds

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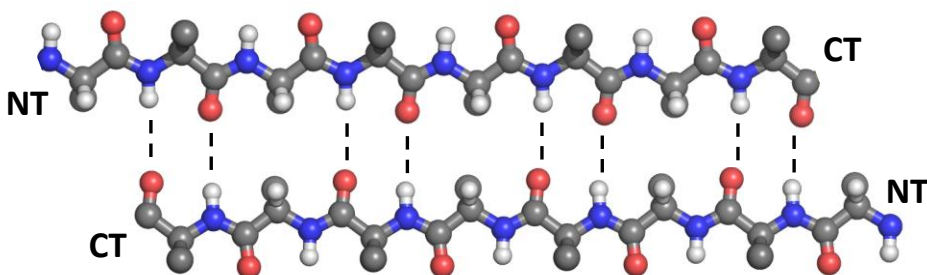
Backbone Hydrogen Bonding



- Beta sheets are made of beta strands
 - No specified hydrogen bonding formula
 - Sheets can form between distant sets of residues
 - **Shown:** Parallel beta sheet

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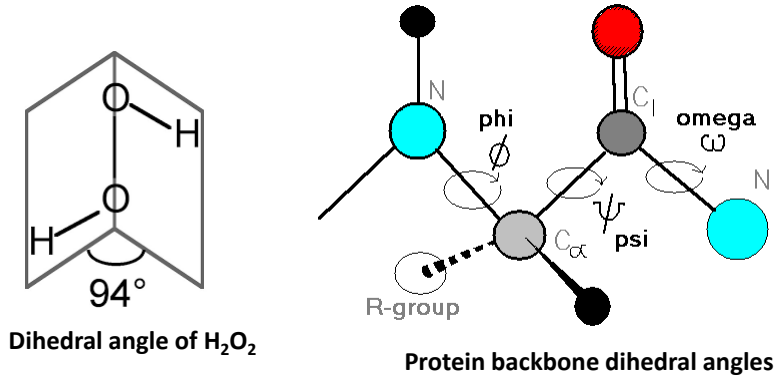
Backbone Hydrogen Bonding



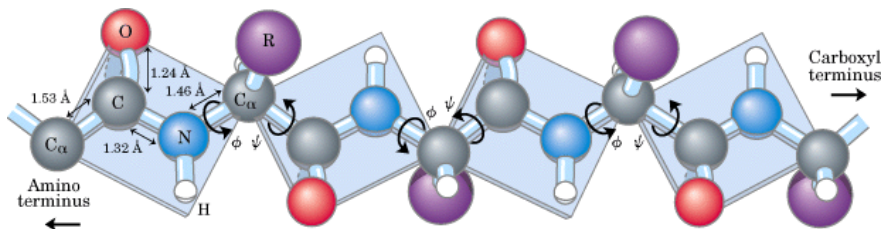
- Beta sheets are made of beta strands
 - No specified hydrogen bonding formula
 - Average ϕ is -120° , Average ψ is 120° (with large variation)
 - Sheets can form between distant sets of residues
 - **Shown:** Antiparallel beta sheet

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Making Sense of the Backbone

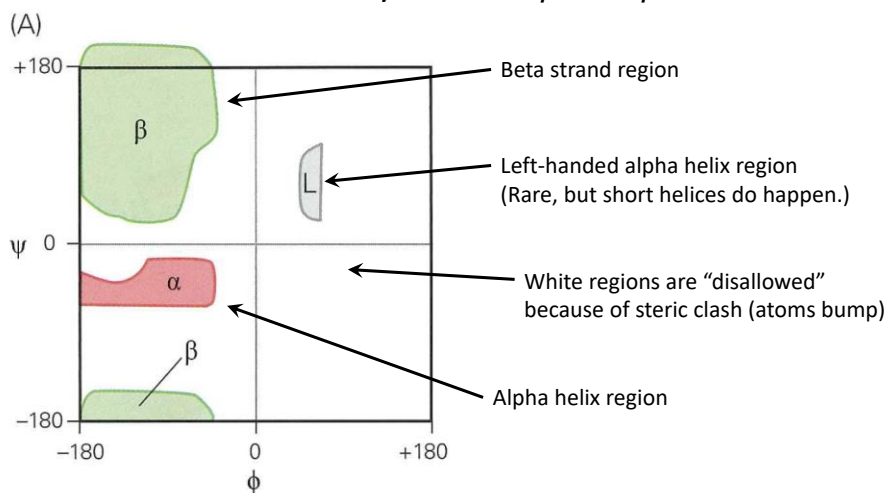


Making Sense of the Backbone



The Ramachandran Plot:

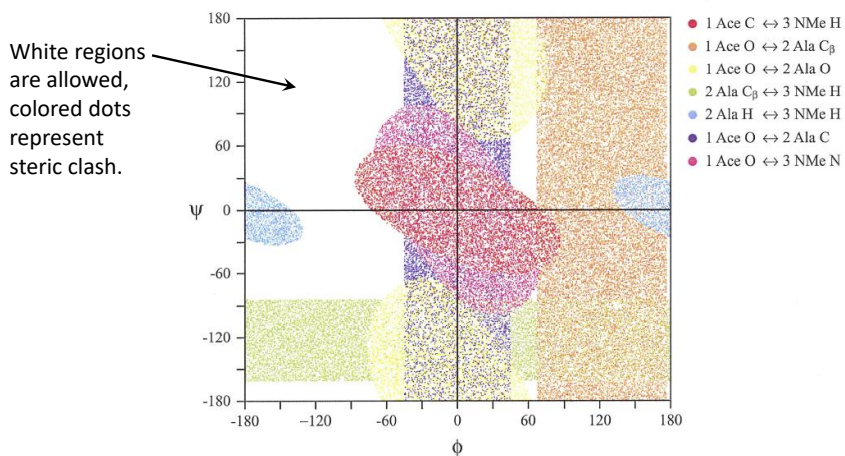
Sterically-allowed ϕ and ψ



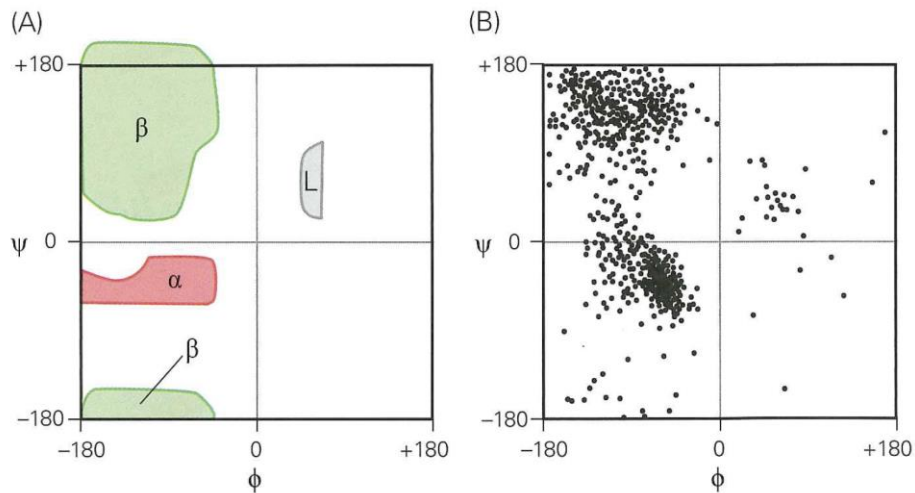
Molecules of Life, pp. 142

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Ramachandran Reversed



Ramachandran Plot – Proteins



Molecules of Life, pp. 142

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Think and Discuss

Why might you see violations to the Ramachandran plot?

Hierarchy of Structure

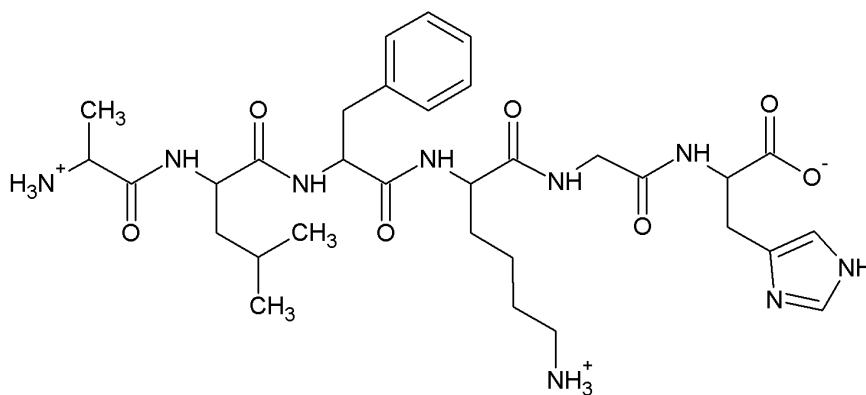
- First proposed by Linderstrøm-Lang



Sources: <http://www.biokemi.org/biozoom/issues/488/articles/1910>
http://en.wikipedia.org/wiki/Carlsberg_Laboratory

23

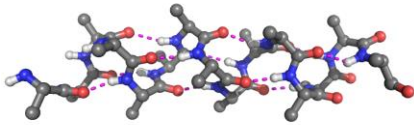
Primary Structure



Think: Sequence of amino acids

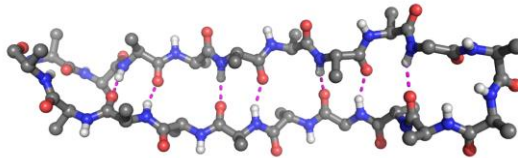
24

Secondary Structure



α Helices

β Strands/Turns



Think: Backbone hydrogen bonding

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Secondary Structure



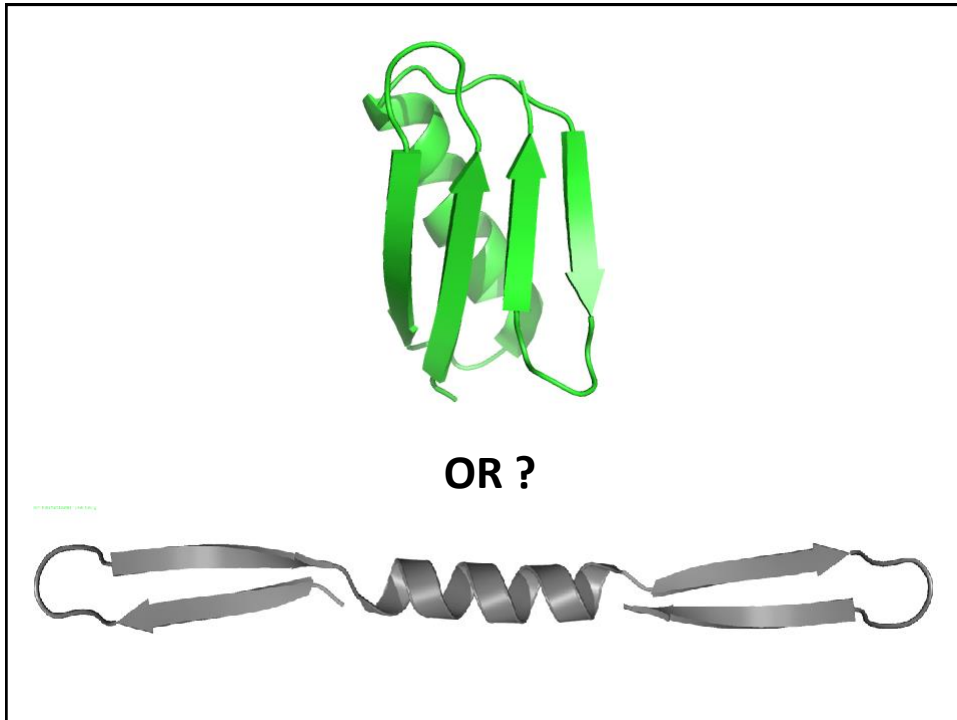
α Helices

β Strands/Turns

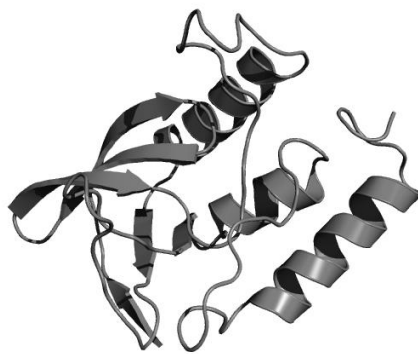


Think: Backbone hydrogen bonding

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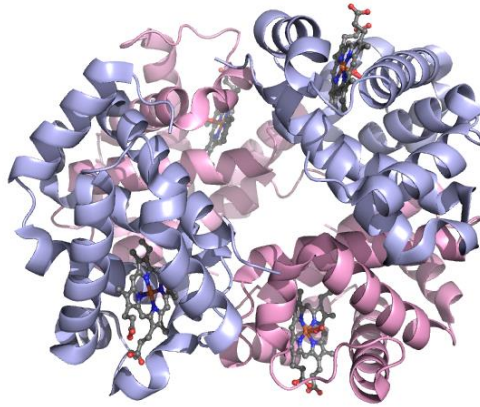


Tertiary Structure



Think: Three-dimensional coordinates

Quaternary Structure



Think: Complexes of multiple proteins

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Think and Discuss

Does it make sense to think about one type of structure being more important than another?

Summary

- Proteins are chemical chains, made up of 20 different amino acids
- The chemical structure of the backbone has consequences: helices, sheets, and turns
- Protein structure is classified into a four-level hierarchy