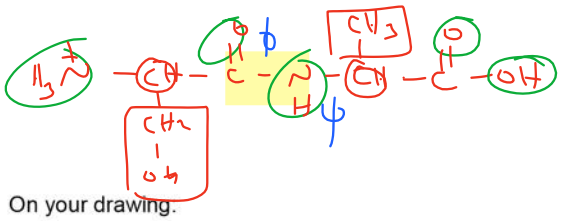
Secondary Structure

1. Draw a dipeptide at pH 7 with the N-terminus to the left and the C-terminus to the right. You may choose any amino acids that you'd like.



2. On your drawing:
   a. Circle the α carbons.
   b. Draw a box around the R-groups.
   c. Circle the atoms capable of H-bonding.
   d. Highlight the atoms involved in formation of the peptide bond.
   e. Label at least one Φ and one Ψ angle.

3. What is the hybridization of the two atoms involved in peptide bonds? If you did not pick sp^3, justify your choice. What is the geometry (you know, linear, trigonal planar, tetrahedral, etc.) around those atoms?

sp^2 b/c of resonance w/ the enol form
trigonal planar

Alpha helix

4. Carefully inspect the image to the right, which shows the backbone atoms in an alpha helix.
   a. Which color stick represents

Carbon gray Oxygen red Nitrogen blue

   b. What do you notice about the position of the backbone carbonyls? What about the backbone nitrogens?

they are all pointed up (C=O) or down (N-H) the ways of the helix

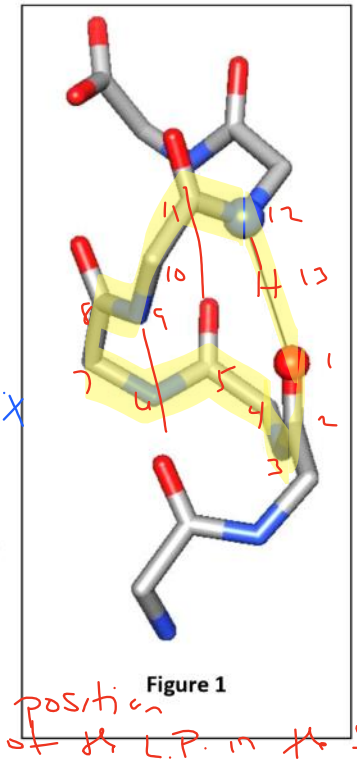


Figure 1

5. Two backbone atoms are shown as a sphere. Based on your answer to 3, draw the hydrogen atom that is missing from the nitrogen.

Does the H-bond appear to be "head on" (that is, lined up directly in the plane of the two atoms)? Think about the position of the lone pairs on oxygen – should the H-bond be "head on"? Why did you choose your answer?

not exactly - the N-H is off center.
Yes, this makes sense b/c of the position of the L.P. in the sp^2 Oxygen

6. Can an H-bond exist between the two sphere atoms? If so, show it. Could similar H-bonds form at any other place in this molecule? If so, label those places.

yes - between all C=O & N-H

7. How many atoms are present in the "ring" that is formed when these two atoms H-bond (make sure to consider the hydrogen)?

highlighted - 13

Use the image to the right to answer questions 8-13.

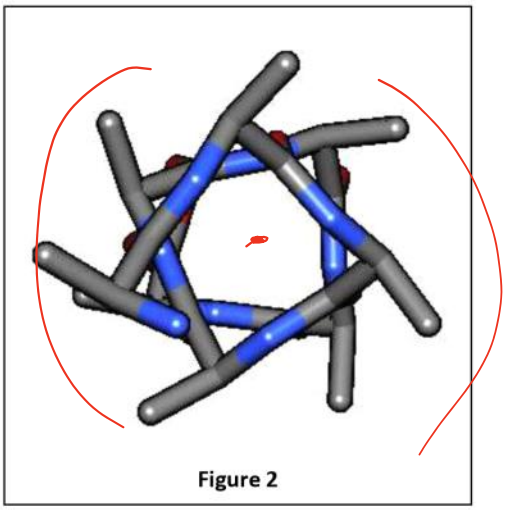


Figure 2

8. Label the central axis of the helix.

9. Label the exterior of the helix.

10. What forms the interior of the helix?

backbone

11. Why are oxygen atoms not easily seen in this image?

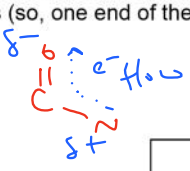
they are pointed directly down

12. Do you think there is any space in the middle of the helix? If so, what do you think will fit there?

No! See spacefill on the next page

13. Think about what you learned about the structure of alpha helices from the last 10 questions. Do you think that alpha helices have a polarity down the central axis (so, one end of the helix is partially positive and the other is partially negative)? Clearly explain your answer.

N-term = δ+
C-term = δ−



Use Figure 3 to answer questions 14 - 19

14. Label the N- and C-termini with "N" and "C"
15. Circle 4 peptide bonds.
16. What intramolecular forces stabilized secondary structure but is not explicitly shown on a ribbon diagram. Be specific – how does this intramolecular force stabilize the structure?

the backbone atoms are not shown, so the H-bonding isn't shown. It's important to remember that it is there!

17. In the last question, IMF was referred to as **intra**molecular, not **inter**molecular as we are used to. Why did I make this change? Do you think that it is an appropriate change? Explain your answer.

Intra means within the same molecule, so yes, this is appropriate

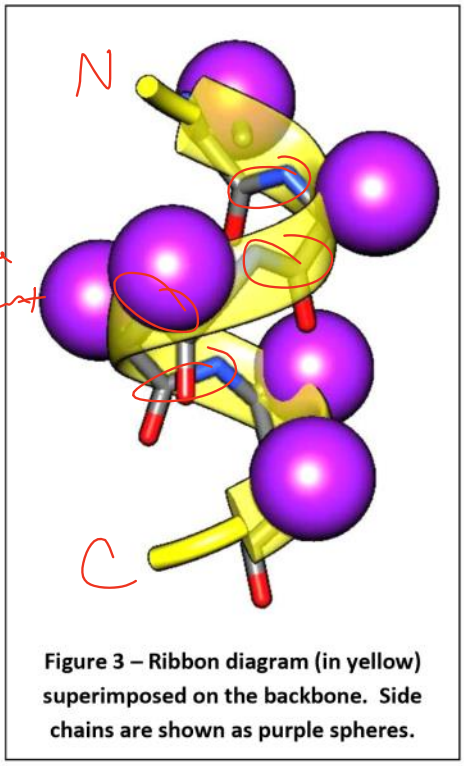


Figure 3 – Ribbon diagram (in yellow) superimposed on the backbone. Side chains are shown as purple spheres.

18. What is missing from ribbon diagrams? Remember that the ribbon diagram is only the yellow part.

Side chain + backbone

19. What does the ribbon reveal about the peptide structure?

it's an alpha helix

20. On the ribbon diagram to the right, starting at 12:00, indicate the position of 4 amino acid side chains.

21. Are these side chains facing the interior or exterior of the helix?

Exterior!

22. Based on this observation, are side chains of alpha helices more important for primary or secondary structure? If not, what role(s) do you think that side chains play in protein structure and function?

No - they are most important for driving 3° + 4° structure interactions

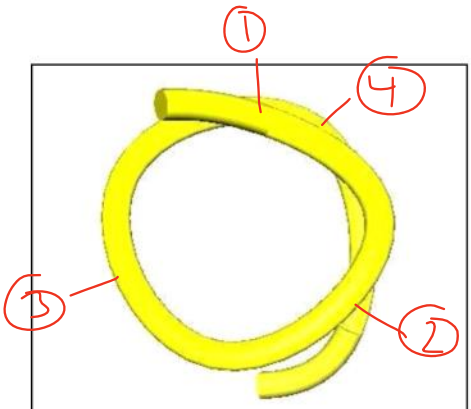


Figure 4 – Protein α-helix ribbon diagram, N-terminus view.

Finally, a space fill image looking down the helical axis is shown below. Based on this, is it possible for a single alpha helix to serve as a pore to allow water to pass through a membrane? Why or why not.

No space!