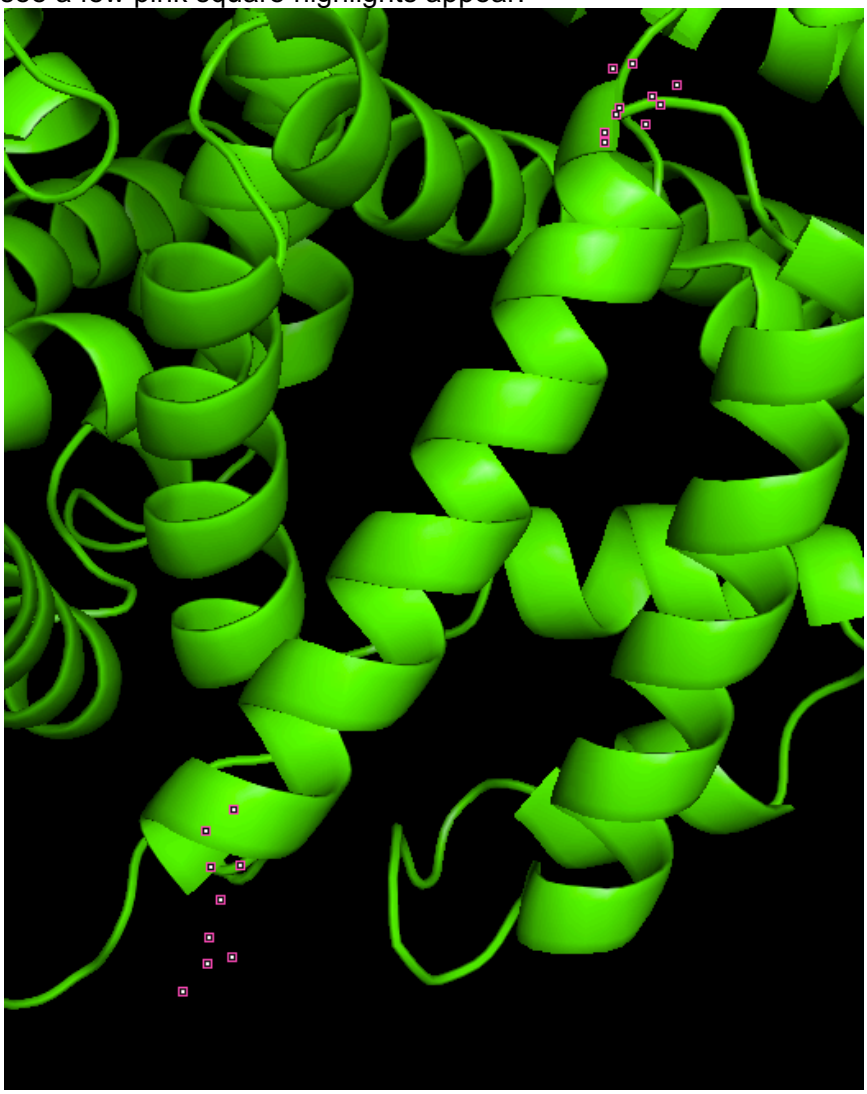
Protein 1° Structure

1. Draw the chemical structure of the peptide with the following sequence *FKIGE.*
2. Indicate each covalent bond that is a peptide bond.
3. Indicate each bond associated with either a Φ or Ψ angle.
4. Determine the pI of the peptide.
    a. Make a table with columns identifying each ionizable group on the peptide and each row indicating a pH from 1 to 14 at 0.5 pH-value intervals.
    b. Fill in the net charge of each ionizable group at each pH value.
    c. Make a final column of the overall charge of the peptide at each pH value (add each individual value).

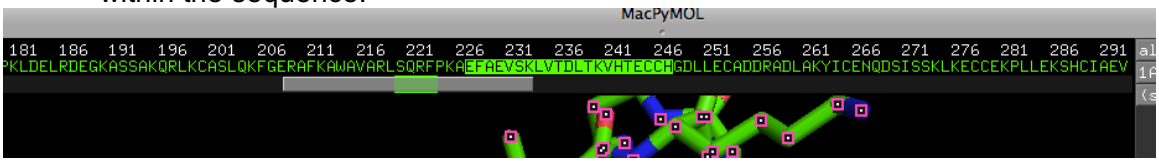
Protein 2° structure

α-helix

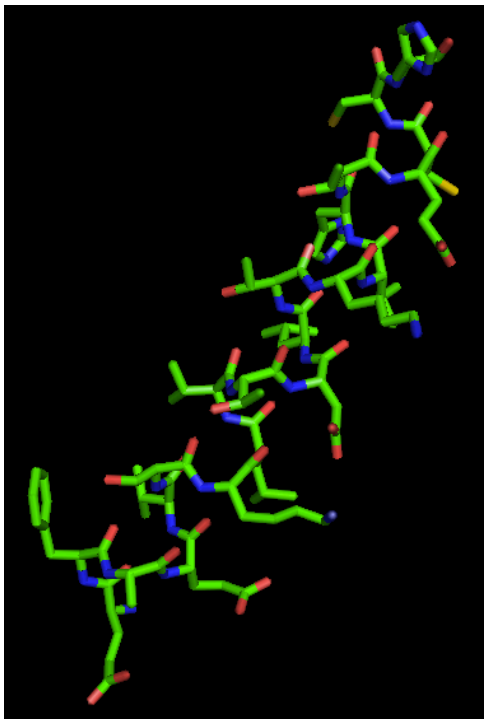
1. Open the structure of Human serum albumin (HSA; 1AO6) in PyMol.
2. Hide everything
3. Show everything as a cartoon
4. Choose an alpha helix by single-left clicking on the beginning and end of a helix. You should see a few pink square highlights appear.



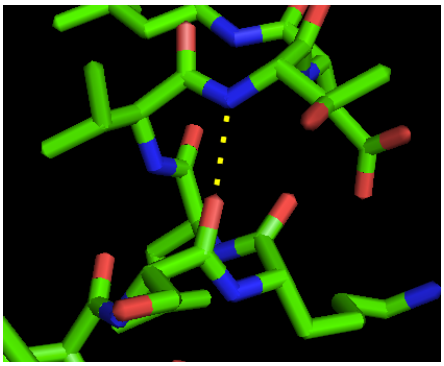
5. Turn the protein sequence “on” under the display tab.
6. Scroll to the region of the sequence that is highlighted. Highlight all the residues of your chosen helix by single-left clicking the residues between the previously selected ends within the sequence:



7. Rename the selected residues by clicking the “action” (A) tab for the (sele).
8. Hide everything
9. Show your helix as sticks



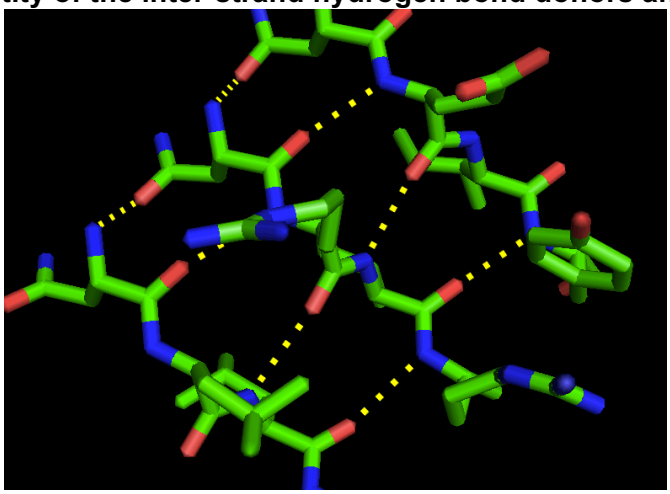
10. **Identify the atom that each color corresponds to.**
11. **What is the relative positioning of the residue side chains compared to the axis of your helix?**
12. Inspect the protein backbone atom sequence to determine the N- and C- termini of your helix. **Is the helix right or left handed from N to C?**
13. PyMol allows you to measure inter-atom distances. Under “Wizard”, select measure. Click on a carbonyl oxygen of the protein backbone with your helix for the first atom. Click on the nearest hydrogen bond donor within your helix that seems to have the correct bond geometry. **What is the chemical identity of the acceptable hydrogen bond donor?**



14. **What is the distance between the hydrogen bond acceptor (carbonyl oxygen) and donor?**
15. **Is this a reasonable distance for a hydrogen bond?**
16. **How many residues are connected between the hydrogen bond donor and acceptor on your helix?**
17. **Approximately, how many residues are there per turn of your helix?**
18. Select and display the helix that comes into closest proximity of your original helix as sticks (method as above).
19. **What chemical functional groups are nearest to each other?**
20. **Are there any covalent linkages between the two adjacent helices?**

Protein Secondary Structure -- β-strands

1. Switch roles with your partner.
2. Open the structure of UDP N-acetylglucosamine acyltransferase (1LXA) in PyMol.
3. Hide everything
4. Show everything as a cartoon
5. The arrows of the beta strands indicate the N- to C- direction of the protein backbone in each strand. **Are adjacent sheets parallel or antiparallel?**
6. Select and display three adjacent beta strands within one beta sheet as sticks.
7. Use the measure wizard tool to determine the distance (and highlight) between every hydrogen bond donor and acceptor pair between each adjacent strand. **What is the chemical identity of the inter-strand hydrogen bond donors and acceptors?**



8. **Describe the hydrogen-bonding pattern of the middle strand.**
9. **Describe the side-chain positioning relative to the "plane" of the beta sheet.**
10. Open the structure of Mannose-specific agglutinin (1JPC) in PyMol.
11. Hide everything
12. Show everything as a cartoon
13. The arrows of the beta sheets indicate the N- to C- direction of the protein backbone in each strand. **Are adjacent sheets parallel or antiparallel?**
14. Select and display the three longest adjacent beta strands of one sheet as sticks.
15. Use the measure wizard tool to determine the distance (and highlight) between every hydrogen bond donor and acceptor pair between each adjacent strand. **What is the chemical identity of the inter-strand hydrogen bond donors and acceptors?**
16. **Describe the hydrogen-bonding pattern of the middle strand.**
17. **Describe the side-chain positioning relative to the "plane" of the beta sheet.**