

Interactions Between 2° Structures

1. Open the structure of Ubibuitin-conjugating enzyme (1U9A) in PyMol
2. Hide everything
3. Show everything as a cartoon
4. Hide everything
5. Show everything as a surface. **Does the surface representation change your perspective on how the secondary structures interact within a protein? How?**
6. Hide everything
7. Show everything as a cartoon
8. Select and display the beta sheet and the helix around which it wraps as sticks and cartoons.
9. **How many polar residues are positioned to interact between the helix and beta sheet?**
10. **How many nonpolar residues are positioned to interact between the helix and beta sheet?**
11. **What type of intermolecular forces dominate the interaction between the helix and the beta sheet?**
12. **How many polar residues of the helix and beta sheet are positioned to interact with the solution around the protein?**
13. **How many nonpolar residues of the helix and beta sheet are positioned to interact with the solution around the protein?**
14. **Explain the observations of #9 through #13.**

3° Structures

Coiled-Coil Domain

1. Open the structure of Leucine zipper GCN4 (2ZTA) in PyMol
2. Hide everything
3. Show everything as a cartoon
4. Select the nonpolar residues from the sequence and show them as spheres.
5. **Where are the hydrophobic residues located?**
6. **Based on your knowledge of the structure of the helix, how would you predict whether a primary sequence would fold into this shape of two coils wrapped around each other (coiled coil)?**

Up-and-Down β Barrel Domain

7. Open the structure of the transmembrane β barrel (2JMM) in PyMol
8. Hide everything
9. Show everything as a cartoon
10. Take in the simple beauty of the fold
11. **Is the wrapped β sheet parallel or antiparallel?**
12. This β barrel forms a pore through which certain materials may pass through the phospholipid bilayer that surrounds cells and organelles. **Use your PyMol skills to estimate the width of the phospholipid bilayer.**
13. **Do you expect to find hydrophobic or hydrophilic residues on the outside of the β barrel?**
14. Under "action" generate a vacuum electrostatic imagine of the barrel.
15. **Does this imagine support your expectation from #27? How?**

Open β Sheet (Rossmann fold)

16. Open the structure of human lactate dehydrogenase M isoform in complex with NADH (4L4S) in PyMol.
17. Hide everything and show residues 21 through 148 as a cartoon.
18. Show the NADH cofactor as spheres.

Protein Quaternary Structures

1. Open the structure of *E. coli* β -galactosidase in complex with allolactose.
2. **How many subunits compose this complex?**
3. **What residues are found at the interface between adjacent subunits?**
4. **What are the chemical properties of the residues found at the interface between adjacent subunits?**
5. **What protein 3° structures can you find?**
6. **Are a majority of β -sheets parallel or antiparallel?**
7. **How many amino acids compose the 1° of each subunit?**