Model Design Parameters

Designing and building a physical model of a protein is not difficult – assuming you have already determined the important features of the protein that you wish to display in the model. As you are reading background papers, you should make a list of important interactions you might consider displaying on your model. Here's a list of some of the features that may be useful to display in your model (not all features are found in every protein!):

- Amino acids involved in binding a substrate or ligand (and any details about which atoms are interacting in the binding)
- Protein cofactors, ATP binding sites, DNA binding sites, etc. – list specific amino acids involved
- Does the protein function in a dimeric (or multimeric) state? If so, do you want to display the dimer? And if you model the dimer, do you want to show different things in the two monomers?
- Are there structural features you want to emphasize in the model?
    - Beta sheets
    - Alpha helices
    - A loop that undergoes a major conformational change when activated
    - Disulfide bonds
    - Individual chains in a multichain protein
    - An unusual gorge or pocket or domain that is important to protein function
    - An amino acid that, when mutated, impacts protein function (may cause disease, or render protein non-functional, or some other impact)
    - Any ligands associated with the protein in your pdb file? (You will need to know how to call these up in Jmol; the pdb webpage will include a list of ligands and their abbreviations)

This list is not intended to be exhaustive, but to give you some ideas about what you might want to display in your model.

Note on identifying amino acids important to protein structure: Jmol uses the three letter abbreviations for amino acids, along with the residue number – such as his404. You should note if interactions are with the amino acid sidechain or with atoms in the backbone. (We use a separate set of commands to show backbone vs. sidechain atoms, and we typically don't display both.)

Prior to the Jmol training session, your team should have generated a list of important features you want to display on your protein model. Once these features are determined, it is possible to finalize your model design in just a couple of hours. For quick reference, you'll find a data sheet below that will help you organize the information you'll need for model design.

PDB file	
Protein Name	
Number of chains and their names (info from pdb website)	

Additional molecules associated with the protein in the file (include name and what it is called in the pdb file)	
Important sidechains, their function (you may list a set of sidechains with a common function)	
Structural features you want to emphasize	
Other features you want to include	