Model Design Parameters

When you build a protein model using a 3D printer, you want the model to be sturdy enough to be handled and you want to highlight interesting features, such as binding sites, catalytic sites, or mutations. Once you have explored your protein and determined the molecular story you want to tell, it will be easier to design a model.

Listed below are some guidelines to assist you in your model design. Please note that not all points in this guideline will be applicable for each model design.

Happy modeling!

Identify the PDB file you will use:

For your qualification model, you will be told which PDB file to use. Your mentor will help you determine the best PDB file to use for your Research and Design model. If you are choosing your own file, some parameters to consider include:

- What organism is the protein from?
- Is the PDB file of the entire protein, or at least the portion of the protein you will model?
- Consider whether the protein exists as a monomer, dimer or other multimer – and what you want to model.
- If you are focusing on a binding site, does the PDB file include the substance (substrate, inhibitor, cofactor, etc.) you want to study?
- What is the resolution of the PDB file? The smaller angstroms indicate better resolution and higher quality data.
- Reading the abstract of the primary citation for the PDB file will also help to identify which PDB file is best if you are wavering among a few files.

Decide which features you want to emphasize as you tell the Molecular Story associated with your protein. You'll get this information from reading the primary citation and associated articles, as well as through discussions with your Mentor:

- Are there important sidechains you want to display?
- What are the sidechains?
- Why are they important?
- Are there important secondary structure features you want to emphasize?
- There are common protein folding motifs that structural biologists have named creatively. Does your protein have one of these structures (it will be discussed in the primary citation) such as a beta barrel, zinc finger, immunoglobulin fold, alpha horseshoe, etc., that you wish to highlight?
- Is there an accessory molecule such as a substrate, inhibitor, cofactor or metal ion that is important to your molecular story?

Determine your color scheme:

The colors that you wish to use should be personal choices, but you should select your choices with a plan in mind to emphasize particular features of your model. Below are a few guidelines to help you in the color selection process.

- If you want to highlight a feature, chose a light color on a dark background OR a dark color on a light background.
- Always select bright or contrasting colors to highlight significant features.

- Avoid using closely related shades of a color to represent different features. The printer may not be able to distinguish the nuances between the shades, creating a model that is essentially the same color throughout.
- Use light colors (white, gray) on less significant features such as hydrogen bonds or monitor lines.
- You might consider using CPK colors on featured sidechains, and color-coding the backbone of these sidechains to indicate different features such as binding sites, catalytic sites, etc.
- Jmol has a great list of colors from which to choose. Please refer to their website for color choices (http://jmol.sourceforge.net/jscolors/).
- Do not use black. This does not print well.

Model Design Specifications:
When designing your model using Jmol, please use the following values to ensure a stable model.

- Backbone 1.5
- Hydrogen bonds 1.0
- Spacefill (in sidechains) 1.25
- Wireframe (in sidechains) 1.0
- Struts 1.0
- Disulfide bonds (1.0

Use hydrogen bonds within beta sheets for stability. Remove the "triangle bonds" – the extra bonds that might appear between amino acid n and amino acid n+2 (ex: Ala5 and Thr7). These bonds exist within a single strand, and do not connect two strands.

Struts
Jmol has a command to add struts based on a defined algorithm that will provide most of the structural supports that you will need. Please note that the "calculate strut" command will not provide all the necessary struts needed for support. For example, the "calculate strut" command does not connect ligands/substrates to the protein. You will need to add those in separately. When reviewing the model to determine the need of strut addition, consider the following:

- Do you have a substrate, cofactor, metal ion or inhibitor? Struts will be needed to connect these ligands to the protein.
- Does your protein have multiple subunits? Review the interface between the subunits to ensure adequate connection points to stabilize the model.
- Check all helices to ensure that they are stabilized by at least one strut. Longer helices will need additional struts.
- Loops and other non-defined regions will need to be stabilized.
- Struts should not exceed 9 angstroms.

Final review of your model
Before submitting your model design to the CBM, review it to make sure that your model

- Does not contain any triangle hydrogen bonds
- Has clean backbones for displayed sidechains (unless backbone atoms have a particular role in the function of the protein)
- Does not have struts that exceed 9 angstroms in length

- Uses bright colors to highlight important features of the protein
- Has light/subdued colors for struts and hydrogen bonds
- Has enough struts to stabilize the protein