Model Design Review

After you have completed your model design, CBM staff will review the model to determine if it is buildable. You may wish to conduct the preliminary review yourself to troubleshoot before submitting your model. Here are the steps:

1) SAVE a jpg of your model design. (Some of the review steps may undo your hard work – but if you have a copy saved, you will lose nothing!)
2) As you go through these steps, there will be points at which you need to watch the model design when you hit enter. These commands appear in bold, followed by what you should watch.
3) Information in brackets indicates variable that you must specify
4) VERIFY BACKBONE SCALE
    a. Select [chains you displayed in your model]
    b. Backbone 1.5
    c. Check that the backbone doesn't change in size when you hit enter. If it does, you need to correct the backbone size in your model. (In rare cases, a different backbone size may be used, but this must be approved by CBM staff.)
    d. To correct:
        i. Select [chains you want displayed in your model]
        ii. Backbone 1.5
5) VERIFY SPACEFILL SCALE
    a. If you are displaying sidechains or substrates or cofactors in ball and stick, you need to check the scale of the balls.
    b. Select [displayed amino acid] and (sidechain or alpha)
    c. **Spacefill 1.25**
    d. Check that the balls on the selected sidechain don't change in size. If they do, you'll need to correct the size.
    e. Compare the size of the balls in the selected sidechain with those of other displayed atoms. Are they all the same size?
    f. To correct:
        i. Select [residue you want to display] and (sidechain or alpha)
        ii. Spacefill 1.25
6) VERIFY PRESENCE OF STICKS IN DISPLAYED SIDECHAINS
    a. Select all
    b. **Spacefill off**
    c. Are all the sidechains you displayed still showing? If some are not, you forgot to use the 'wireframe 1.0' command. If you build a model showing ball and stick sidechains…and you only display the balls (spacefill) and not the sticks (wireframe), it may LOOK fine on the screen, but it will BUILD as a bunch of detached balls.
    d. Are all the sidechains attached to the backbone? If some are not, you forgot to use the 'and alpha' portion of the select command.
    e. To correct:
        i. Go back to your saved version
        ii. Select [residue you want to display] and (sidechain or alpha)
        iii. Spacefill off
        iv. If the sidechain disappears or the sidechain isn't attached to the backbone, use the command: wireframe 1.0
        v. Spacefill 1.25

vi. Repeat for each residue you want to display, as well as cofactors and substrates

f. To avoid:
    i. Once you select what you want to display using the select command:
    ii. Wireframe 1.0
    iii. Spacefill 1.25

7) VERIFY SMOOTH BACKBONE
    a. Select [chains you display in your model]
    b. Backbone 0.7
    c. Look at backbone for each of the sidechains you are displaying. There should be only a single ball displayed on the backbone – right at the bend at which the sidechain attaches. If there are additional balls displayed on either side of this attachment point, you have a bumpy backbone you have to remove.
    d. To correct if only one or two sidechains are bumpy:
        i. Select [chain and residue]
        ii. Wireframe off
        iii. Spacefill off
        iv. Select [chain and residue] and (sidechain or alpha)
        v. Wireframe 1.0
        vi. Spacefill 1.25
    e. To correct if MANY or ALL of the sidechains are bumpy:
        i. Select backbone
        ii. Spacefill off
        iii. Wireframe off
    f. To avoid:
        i. When selecting a sidechain to display:
        ii. Select [chain and residue] and (sidechain or alpha)
        iii. Wireframe 1.0
        iv. Spacefill 1.25

8) COLOR SCHEME
    a. Look at the model design.
    b. What colors pop out?
        i. These should be colors for the parts of the model you are emphasizing.
    c. What colors are almost invisible – that is, easy to ignore?
        i. These should be the colors you use on the hydrogen bonds, struts, and any other feature you don't want to emphasize.
    d. Are there two colors that are really similar…but that you want to distinguish in the model?
        i. A good test as to whether two colors can be distinguished is to print a copy of the jpg. On the printed page, can the colors be distinguished? If not, choose one color that is more different.

9) HBONDS
    a. Does your structure include beta sheets?
        i. If so, are there hydrogen bonds in the sheets?
        ii. To add hydrogen bonds:
            1. Select sheet
            2. Hbonds on
            3. Hbonds 1.0
            4. Color hbonds white [or some other unobtrusive color]
            5. Set hbonds backbone

b. Look for “floating” hydrogen bonds
    i. These are bonds that are present, but aren’t connected to the backbone. If they aren’t connected, they will build as separate rods – which won’t add any support to your model!
    ii. To correct:
        1. Set hbonds backbone
c. Search for “triangle” bonds
    i. Sometimes when the software calculates hydrogen bonds, the algorithm will incorrectly create a hydrogen bond between two amino acids within a beta sheet that are in the position N and N + 2.
    ii. These hydrogen bonds, in conjunction with the backbone, form a triangle – hence the name “triangle bond”
    iii. Triangle bonds don’t add strength to the model and they detract from the structure, so all triangle bonds should be removed
    iv. Here’s a quick way to spot triangle bonds (make sure you have a saved copy of your model, because these instructions will destroy the model!!)
        1. Select all
        2. Spacefill off
        3. Wireframe off
        4. Restrict sheets
        5. Color hbonds [some bright color that contrasts with your backbone]
        6. Then just rotate the model to see both sides of the sheets and look for hbonds running along the chain. If you find one (fortunately they are rare, but should still be found!)
            a. Click on the two ends of the hbond to identify residue numbers
            b. Make a list of these pairs [for simplicity, let’s call them A and B]
            c. Once you have found them all, go back to your beautifully saved model and use the following commands:
            d. Select [A or B]
            e. Hbonds off

10) STRUTS
    a. Did you add struts to your model?
        i. If not:
            1. Select all [or restrict to the chains you are modeling]
            2. Calculate struts
            3. Struts 1.0
            4. Color struts white [or some other unobtrusive color]
    b. Does your model have a substrate or cofactor? If so, did you attach it to the protein using struts (separate from calculating stuts command)?
        i. Click on the two atoms you want to join with a strut. Jmol will print the atomno for each atom you clicked on.
        ii. Select atomno=[insert one atom number] or atomno=[insert other atom number]
        iii. Connect strut
        iv. Strut 1.0
        v. Color strut white
11) Once you are satisfied that your model is ready to go, send a copy of the jpg as well as the pdb file to CBM staff for final review.