

Guide to Using the Rubric to score the Calmodulin Prebuild Model for Science Olympiad Regional Competitions

These instructions are to help the event supervisor and scoring judges use the rubric developed by the Center for BioMolecular Modeling in scoring the 2008 Science Olympiad Regional pre-build Mini-Toober models of Calmodulin, based on 1CCL.pdb. Each category on the rubric is addressed within these instructions and is accompanied by a short description and picture, if appropriate.

Overview of the molecule

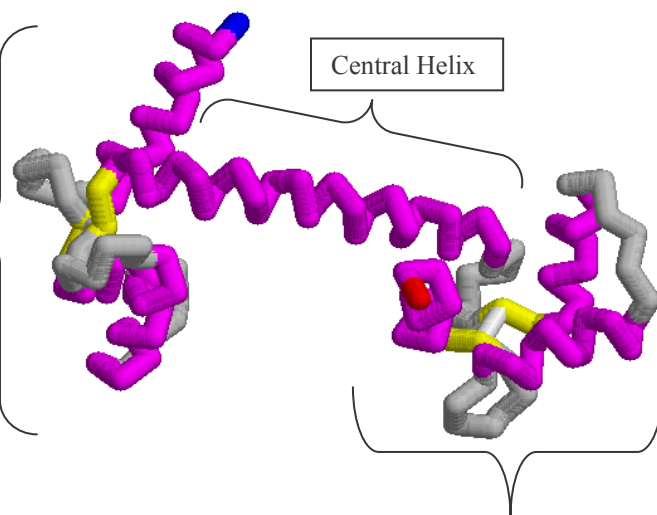
There are three main parts to this molecule, which gives rise to a “dumbbell” shaped protein:

- N-terminus calcium binding domain
- Central helix
- C-terminus calcium binding domain

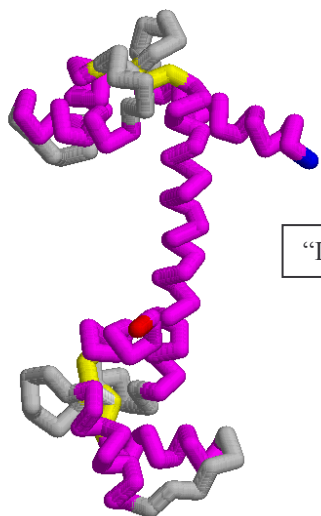
Color Code

Magenta – helices
Yellow – beta strands
Blue tip – N-terminus
Red tip – C-terminus

N-terminus calcium binding domain



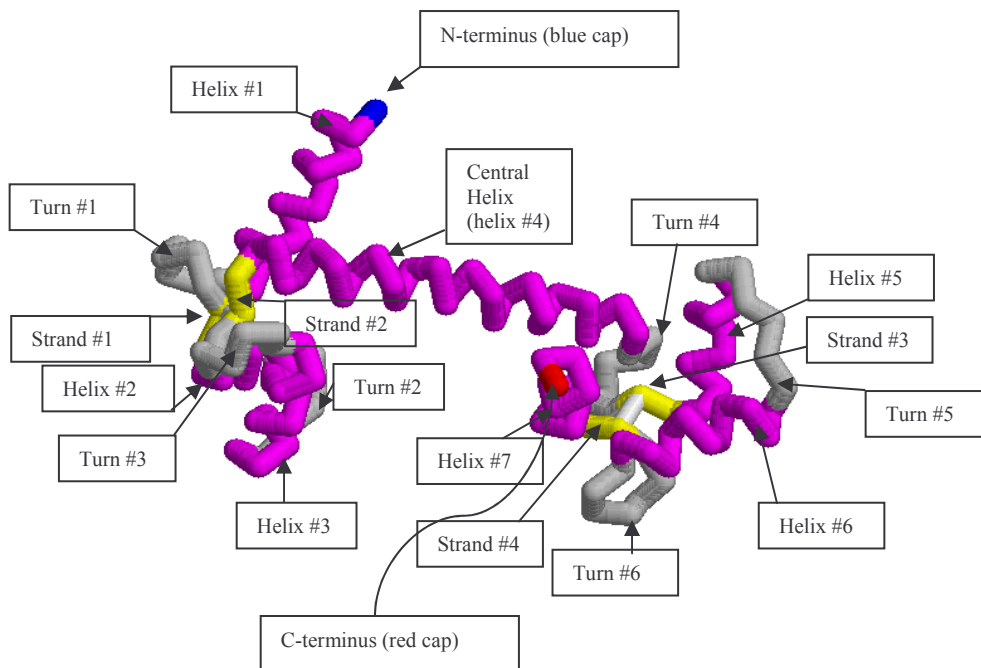
C-terminus calcium binding domain



“Dumbbell” shaped protein

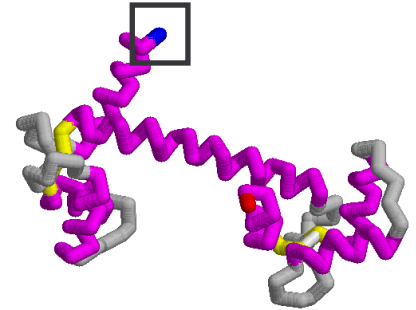
Order of structures:

N-terminus
Helix#1
Turn#1
Beta-strand #1
Helix #2
Turn #2
Helix #3
Turn #3
Beta-strand #2
Central helix (helix #4)
Turn #4
Beta-strand #3
Helix #5
Turn #5
Helix #6
Turn #6
Beta-strand #4
Helix #7
C-terminus



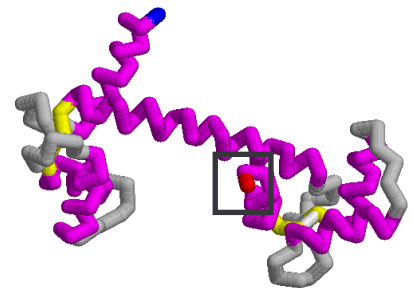
1. Blue Cap on N-terminal Amino Acid (Leu4)

- To receive two points, the blue cap needs to be located at the N-terminus of the protein, which is the beginning of the first helix of the protein. Please see the figure to the right for the correct positioning of the blue end cap.



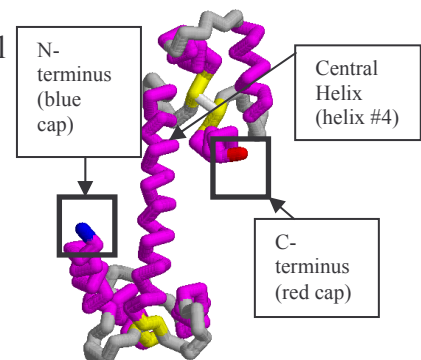
2. Red cap on C-terminal Amino Acid (Ala147)

- To receive two points, the red cap needs to be located at the C-terminus of the protein, which is the end of the last helix. Please see the figure to the right for correct positioning of the red end cap.



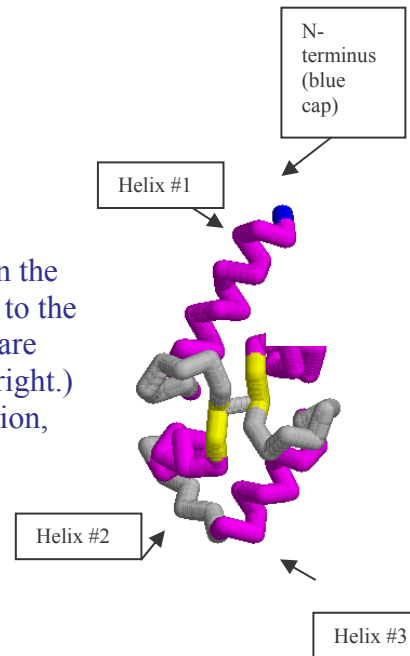
3. N and C termini are located on opposite sides of the axis of the central helix.

- To receive two points, the blue cap and the red cap need to be on opposite sides of the central helix. If holding the model so that the N-terminus is on the bottom and to the left of the central axis (see figure to the right) and the C-terminus is on the top, then the red cap should be to the right of the axis of the central helix. Please see the figure to the right for positioning of the caps.

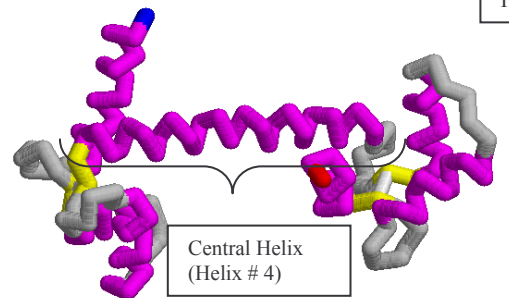


4. Model has 7 alpha helices according to Jmol/RasMol selection criteria

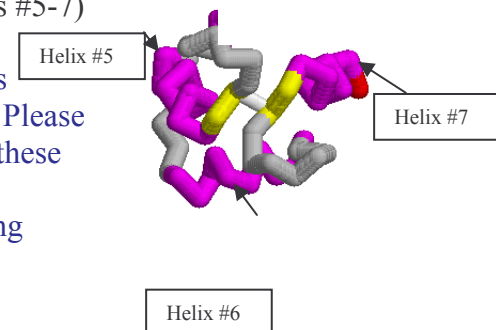
- 3 helices in N-terminus calcium binding domain (helices #1-3)
 - To receive these points, there should be 3 helices within the N-terminus calcium binding domain. Please see figure to the right for the correct location of these helices. (Helices are colored magenta on the model and on the figure to the right.)
 - If there are three helices present, but in the wrong location, award 0.5 point per helix.



- One long central helix (helix #4), which is located between two calcium binding domains of the protein
 - To receive this point, there should be a long helix, connecting the N-terminus calcium binding domain to the C-terminus calcium binding domain.



- 3 helices in C-terminus calcium binding domain (helices #5-7)
 - To receive these points, there should be 3 helices within the C-terminus calcium binding domain. Please see figure to the right for the correct location of these helices.
 - If there are three helices present, but in the wrong location, award 0.5 point per helix.

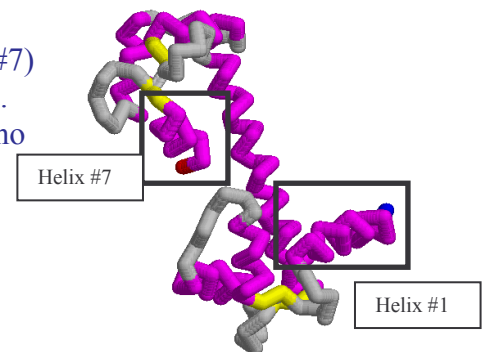


5. Alpha helices are right-handed

- Alpha helices are right-handed. Check each alpha helix in the model to confirm that the helix is right-handed. For each right-handed helix, the model should receive 1 point, for a total of 7 points if all seven helices (Helix #1-7) are correct.
- To determine if the helix is right-handed, find one of the ends of the helix and imagine that the helix is a spiral staircase. Pretend that you are climbing that staircase and you need to have a hand-rail and the helix is the hand-rail, which is always on the outside edge of the staircase. If you would put your right hand on the toober as you go up the staircase, you have a right-handed helix. If you would put your left hand on the toober, you have a left-handed helix and the modeled helix would not receive the point.

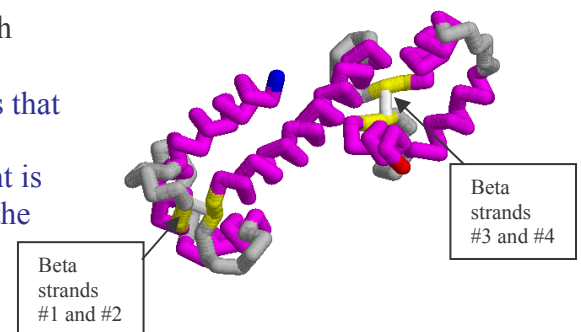
6. C-terminal helix is shorter in length than N-terminal helix

- To receive this 0.5 point, the helix at the C-terminus (helix #7) should be shorter than the helix at the N-terminus (helix #1). Helix #1 is 16 amino acids in length and Helix #7 is 10 amino acids in length.



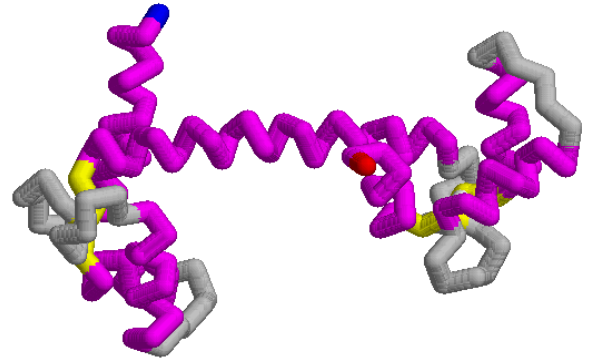
7. Model has one beta sheet (comprised of 2 strands) on each calcium binding domain

- To receive these points, there should be 2 strands that make up the beta sheets in each calcium binding domain section of the model. Each strand present is worth 1 pt. (Beta strands are colored yellow on the model and on the figure to the right.)



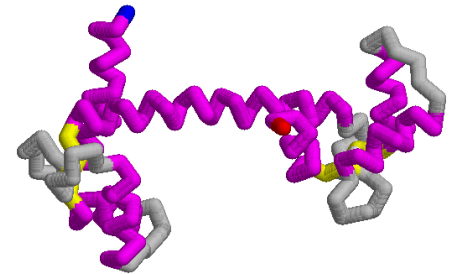
8. Model is dumbbell-shaped (one binding domain on either side of the central helix)

- To receive these points, the model should have a globular domain at each end of the central helix. The model should resemble a dumbbell in that it has two “globular domains” connected by a central helix (or post).



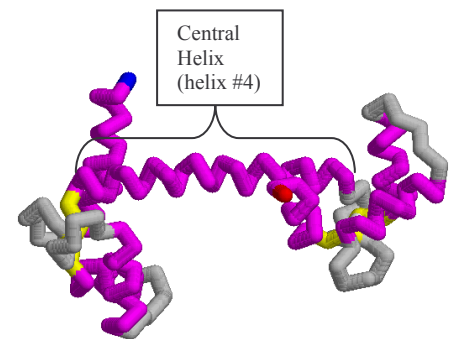
9. Calcium binding domains should be very similar to one another in terms of structure

- To receive this point, the two ends of the model should look very similar to one another. They are essentially the same domain in terms of order of the secondary structures. When looking at the model, the two domains should look the same. To receive this point, there should be very little difference between the two ends. The orientation of the two domains is different from one another, however.



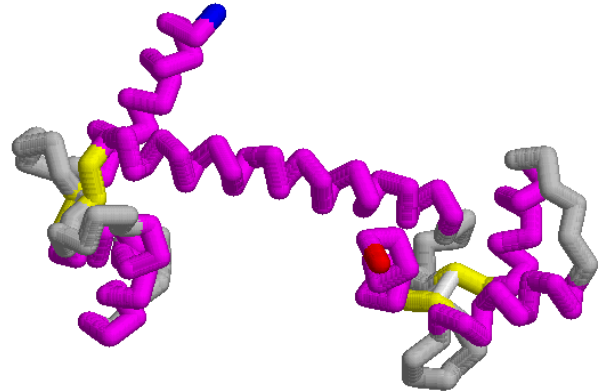
10. Central helix is longer than any other helix in the model (27 amino acids versus 8-16 amino acids)

- To receive this point, the central helix that connects the two calcium binding domains should obviously be the longest helix within the model. Helices 1-3 and 4-7 should be significantly shorter than the central helix.



11. Positioning of secondary structures in the proper order

- To receive these points, the sequence of the secondary structures should be in the following order:
 - N-terminus→Helix#1→Turn#1
 - β-strand#1→Helix #2→Turn#2
 - Helix#3→Turn#3→Strand#2
 - Central Helix
 - Turn#4→β-strand#3→helix#5
 - Turn#5→Helix#6→Turn#6
 - β-strand→Helix#7→C-terminus

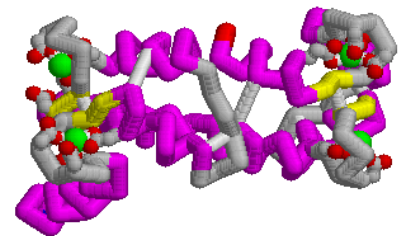


12. Students submitted a 3x5 card with explanation of the model

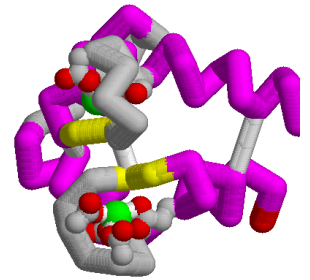
- The 3x5 card submitted with the model should describe the model in terms of what additional features have been added to the model so that the judge is not left guessing what the model represents.

13. Creative additions to the model

- Four calcium ions positioned within the model. There are 2 calcium ions per binding domain (as binding domain is defined in this guide to the rubric; one at the N-terminus with 2 calcium ions and one domain at the C-terminus with 2 calcium ions). Calcium ions are the green spheres in the figure to the right.

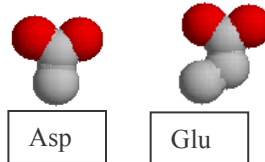


- Amino acids involved in coordinating the calcium ions are displayed (3 Aspartic acid amino acids and 1 glutamic acid amino acid per calcium ion). Oxygen atoms of the amino acids should be facing the calcium ion binding pocket, rather than out away from the model.

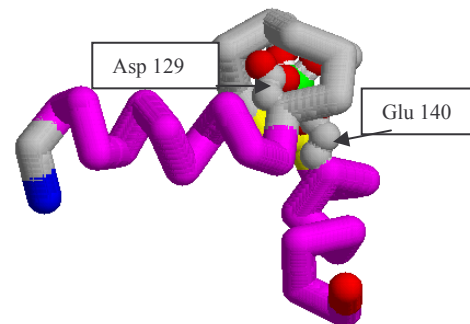
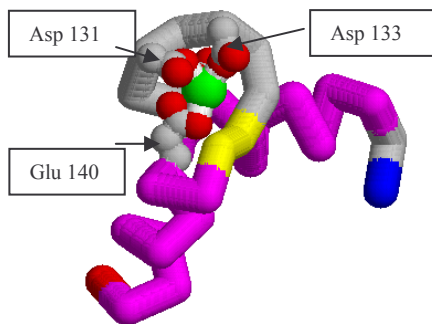


- The 4 amino acids should be positioned appropriately:

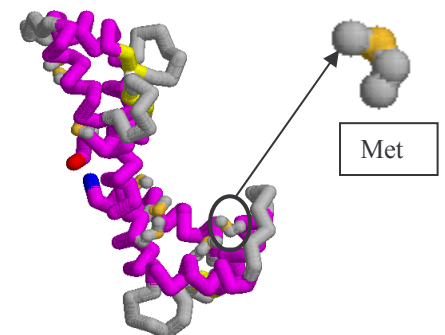
- Asp 129
- Asp 131
- Asp 133
- Glu 140



- The aspartate residues are located at every other amino acid position (129, 131 and 133) and these are positioned on the loop region. The glutamate residue should be located farther from the aspartate residues (at position 140) and the only one to be positioned on the helix. The green sphere in the figure and the model represents the calcium.



- Hydrophobic patches on each binding domain for target protein to bind. As described in Goodsell's Molecule of the Month, there are hydrophobic regions that are important for binding target proteins and these are especially rich in methionine residues (as shown in the picture to the right; these amino acids are not shown on the model).
- Target protein associated with calmodulin. As described in Goodsell's Molecule of the Month, calmodulin interacts with target proteins, including, but not limited to, the edema factor from anthrax, calmodulin-dependent protein kinase II-alpha, and myosin light chain kinase.



- Any other added features that help to tell the story
 - To receive these points, the model should have more to it than just the toober we provided. Listed above are suggestions for inclusions that might appear based on Goodsell's Molecule of the Month.
 - Additional features that are explained (in the abstract or labeled on the model) that help to tell the story are also okay.

14. Creative additions are accurate

15. Creative additions are important to functional importance