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

(Amino Acids 116-147)

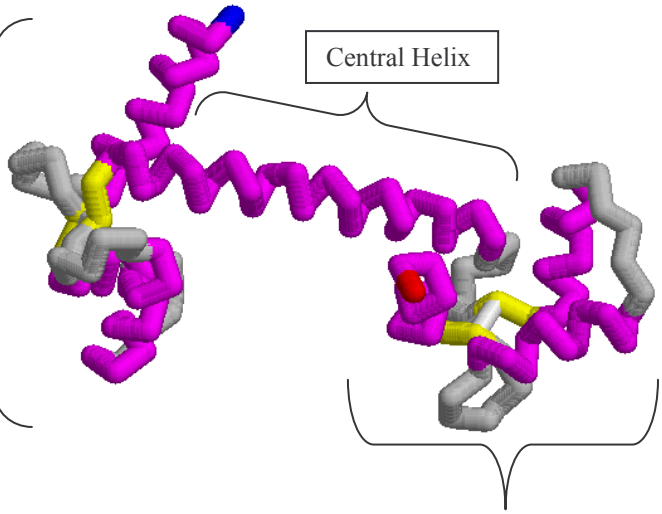
These instructions are to help the event supervisor and scoring judges use the rubric developed by the Center for BioMolecular Modeling in scoring the 2008 Science Olympiad Regional on-site Mini-Toober models of the calcium binding domain of Calmodulin (amino acids 116-147), based on 1CLL.pdb. Each category on the rubric is addressed within these instructions and is accompanied by a short description and picture, if appropriate.

Overview of the entire calmodulin protein

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

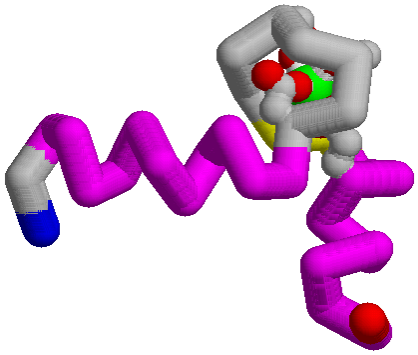
- N-terminus calcium binding domain
- Central helix
- C-terminus calcium binding domain

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



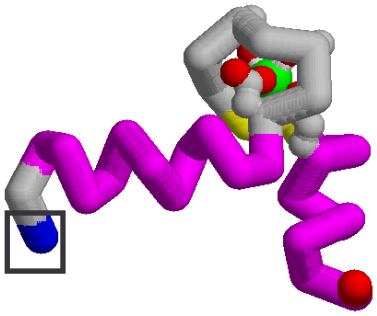
Calcium binding pocket created by amino acids 116-147 (the last 32 amino acids of the protein)

The Regional On-site Model will resemble only this portion of the protein.

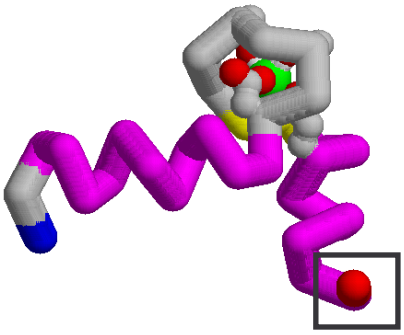


Calcium binding pocket created by amino acids 116-147

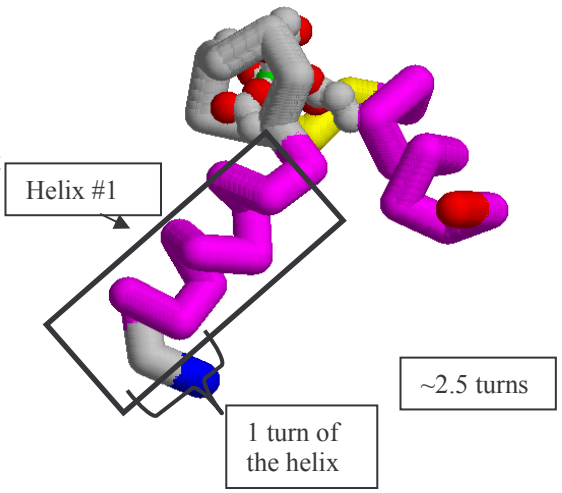
1. Blue Cap on N-terminal Amino Acid (Leu116)
    - To receive two points, the blue cap needs to be located at the N-terminus of the protein. This helix should NOT be located next to the beta-strand. The C-terminal helix is adjacent to the beta-strand. The N-terminal helix should be next to the loop region. Please see the figure to the right for the correct positioning of the blue end cap.



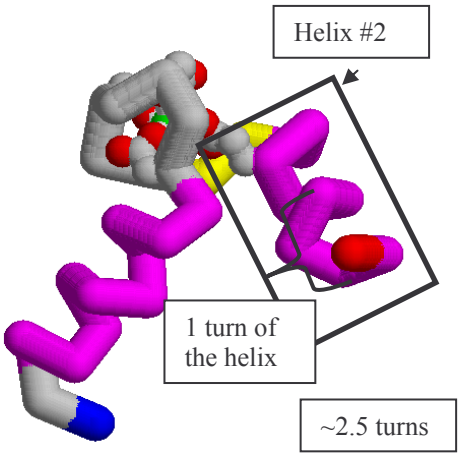
2. Red cap on C-terminal Amino Acid (Ala147)
    - To receive two points, the red cap needs to be located at the C-terminus of the protein, which is the end of the last helix. The C-terminal helix should be adjacent to the beta-strand and NOT the loop. The N-terminal helix should be next to the loop of this region. Please see the figure to the right for correct positioning of the red end cap.



3. Alpha helix #1: Asp118-Ala 128.
    - To receive two points, there should be an alpha helix at the beginning of this protein that is 11 amino acids in length. This helix should have ~2.5 turns to it. Please see the figure to the right to locate the helix. The helices are colored magenta in the figure and on the model.

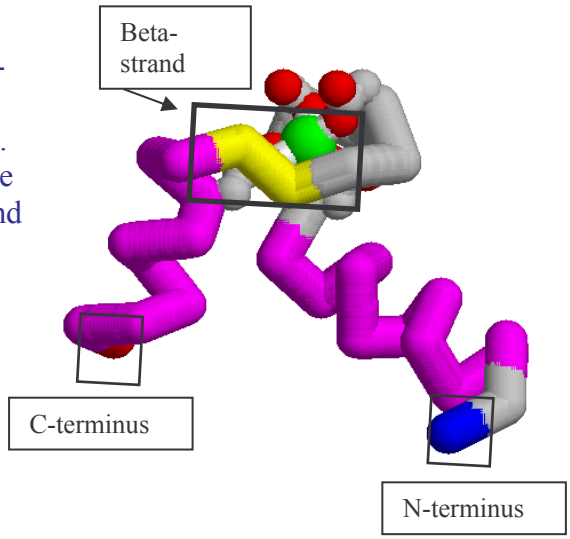


4. Alpha helix #2: Thr138-Ala147.
    - To receive two points, there should be an alpha helix at the end of this protein that is 10 amino acids in length. This helix should have ~2.5 turns to it.



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 2 points, for a total of 4 points if both helices (Helix #1 and #2) 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 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, your 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 points.

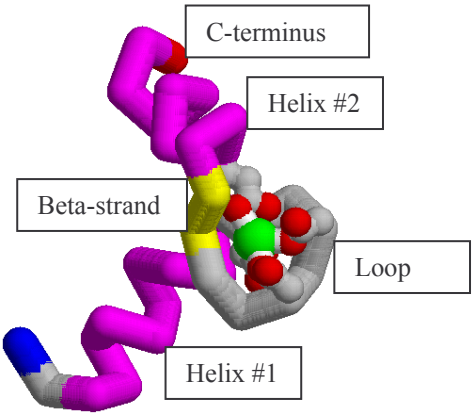
6. Beta-strand: Val136-Asn137
    - To receive these 2 points, there should be a beta-strand located at amino acids 136 and 137. This strand should then lead into the C-terminal helix. Preceding the beta-strand is the loop area. Please see the figure on the right to locate the beta-strand within the model. The beta-strand is colored yellow on the figure and on the model.



7. Correct Topology

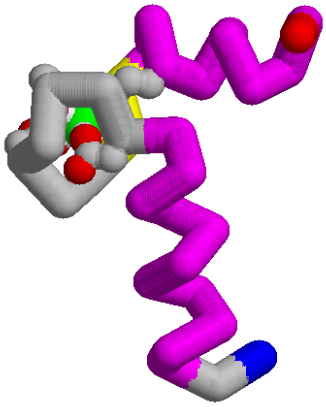
Positioning of secondary structures in the proper order

- To receive these points, the sequence of the secondary structures should be in the following order:
  - N-terminus→Helix#1
  - Loop (turn)
  - β-strand
  - Helix #2-C-terminus



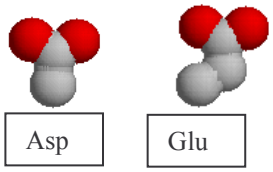
8. Correct 3-dimensional positioning of helices relative to one another

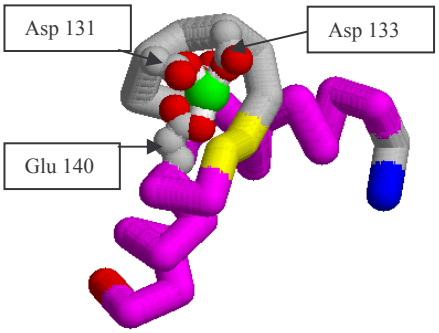
- To receive these points, the helices should be positioned so that they form a sort of "T" shape. The N-terminal helix should lie perpendicular to the C-terminal helix. With reference to the "T" shape, the N-terminal helix should form the bottom part of the "T" and the C-terminal helix should cross at the top.



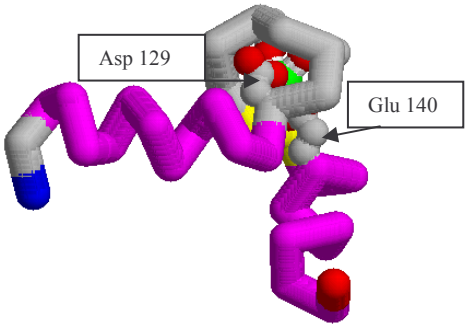
9. Correct positioning of the 4 amino acids that were provided

- To receive these points, the 4 amino acids should be positioned appropriately:
  - Asp 129
  - Asp 131
  - Asp 133
  - Glu 140



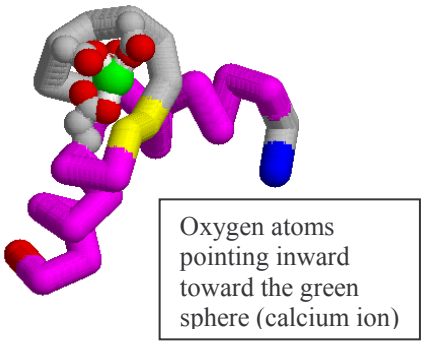


- The aspartate residues are located at every other amino acid position (129, 131 and 133) and these are positioned on the loop region. The glutamate residue should be located farther from the aspartate residues (at position 140) and the only one to be positioned on the helix. The green sphere in the figure and the model represents the calcium (students will most likely NOT have this in their model as no ion was provided to them).



10. Oxygen atoms from 4 amino acids facing the calcium binding "pocket" (facing inward toward the "pocket region" rather than outward.

- To receive these points, the 4 amino acids (Asp129, Asp131, Asp133 and Glu140) should be facing the "pocket region" to which calcium would bind. These amino acids should not be facing outward toward the outer surface of the protein. If you were to put a calcium ion between these 4 amino acids, it should stay.



11. Calcium binding domain located in “pocket” created by the beta-strand and loop

- To receive these points, there should be a “pocket” into which a calcium ion could bind located near the beta-strand and loop region. The amino acids should be positioned in this area. A definite “pocket” should be present. You should be able to imagine a calcium ion binding within this “pocket”. The loop and beta strand should not be far away from each other to create a large gap, but they should be close together to form a region to which a calcium ion could bind.