

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

## (Amino Acids 4-80)

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 amino acids 4-80 of the calmodulin protein, 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

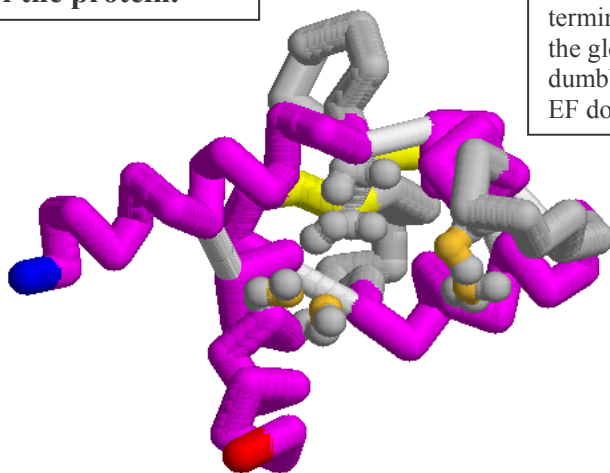
N-terminus calcium binding domain

Central Helix

C-terminus calcium binding domain

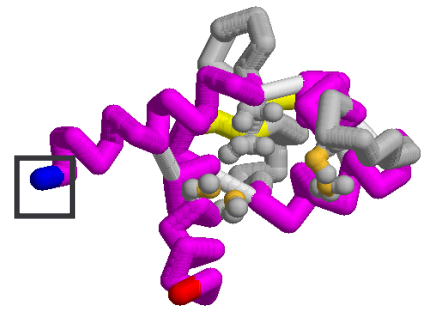
**The State On-site Model will resemble only this portion of the protein.**

Amino Acids 4-80 – The N-terminus of the protein (one of the globular ends of the dumbbell) – contains 2 of the 4 EF domains.



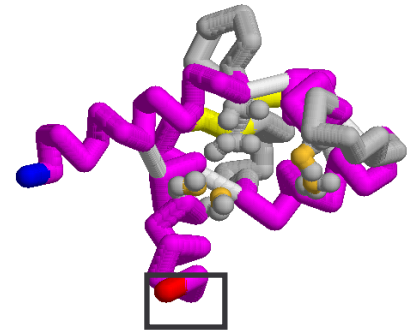
### 1. Blue Cap on N-terminal Amino Acid (Leu4)

- To receive two points, the blue cap needs to be located at the N-terminus of the protein. The N-terminal helix should be next to the loop region. This helix should NOT be located next to the beta-strand. The C-terminal helix is adjacent to the beta-strand. Please see the figure to the right for the correct positioning of the blue end cap.
- Two of the 4 methionines positioned on the model will be located on the C-terminal helix, so the blue cap should be on the helix without any sidechains on it.



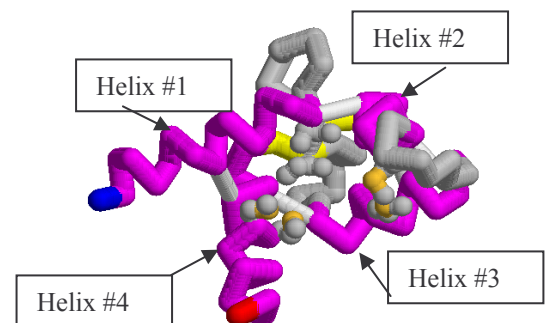
### 2. Red cap on C-terminal Amino Acid (Asp80)

- 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.
- Two of the 4 methionines are positioned on the C-terminal helix, so the red cap should be on the helix with these amino acids on it.



### 3. Model has 4 helices

- To receive points, there should be 4 helices within this model. One point for each helix

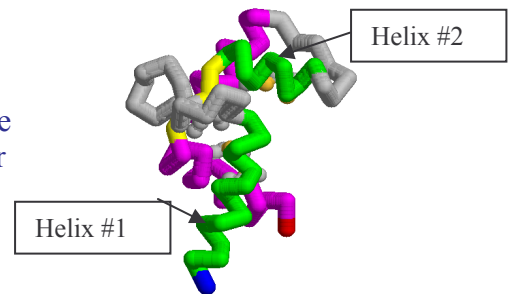


#### 4. Alpha helices are right-handed

- 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 4 points if all 4 helices are right-handed. Please note that it is common to find a combination of right- and left-handed helices within the same model. Therefore, please take the time to check that each helix is right-handed.
- 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 toobar as you go up the staircase, you have a right-handed helix. If you would put your left hand on the toobar, you have a left-handed helix and the modeled helix would not receive the points.

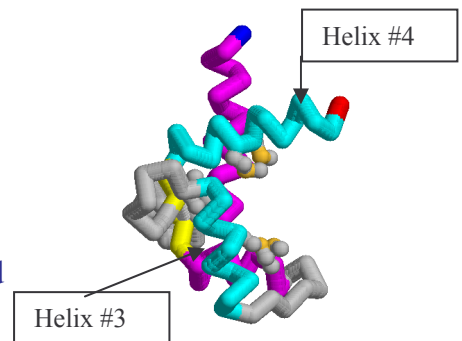
#### 5. Helices #1 and #2 are roughly perpendicular to one another (EF Domain #1)

- To receive these 2 points, helices #1 and #2 should be perpendicular to one another. These two helices form EF-Domain #1 of the this region of the protein.
- Helices #1 and #2 are colored green in the picture to the right. Note that these helices are roughly perpendicular to one another.
- If the helices are parallel to one another, no points should be awarded. If the helices are more perpendicular than parallel, but not quite perpendicular, 1 pt should be awarded.



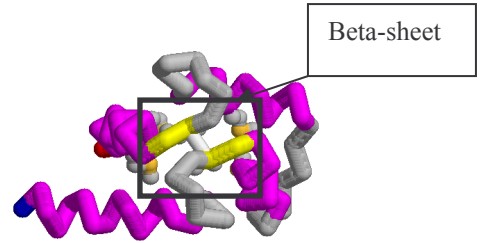
#### 6. Helices #3 and #4 are roughly perpendicular to one another (EF Domain #2)

- To receive these 2 points, helices #3 and #4 should be perpendicular to one another. These two helices form EF-Domain #1 of the this region of the protein.
- Helices #3 and #4 are colored cyan in the picture to the right. Note that these helices are roughly perpendicular to one another.
- If the helices are parallel to one another, no points should be awarded. If the helices are more perpendicular than parallel, but not quite perpendicular, 1 pt should be awarded.



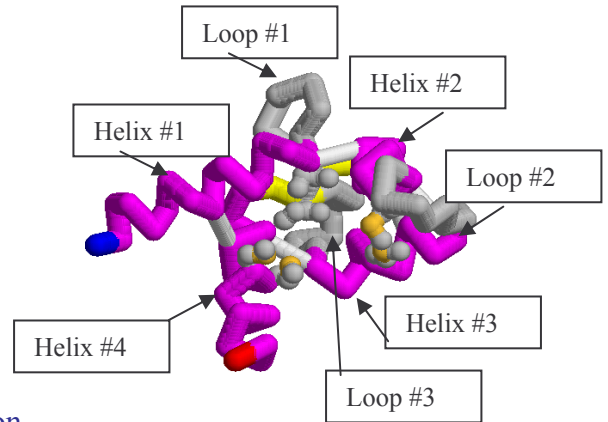
**7. Model has one beta-sheet**

- To receive these 2 points, the model should have a beta sheet within it. This sheet is comprised of two beta-strands, one from each EF Domain.



**8. 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 #2 (turn) / β-strand #1 (the differentiation on the model between these two may be challenging since the beta strand is only 2 amino acids in length, therefore, they are combined for 0.5 pt)
  - Helix #2
  - Loop #2
  - Helix #3
  - Loop #3 / Beta-strand #2 (the differentiation on the model between these two may be challenging since the beta strand is only 2 amino acids in length, therefore, they are combined for 0.5pt)
  - Helix #4 → C-terminus



**9. Correct positioning of the 6 amino acids:**

4 Methionine

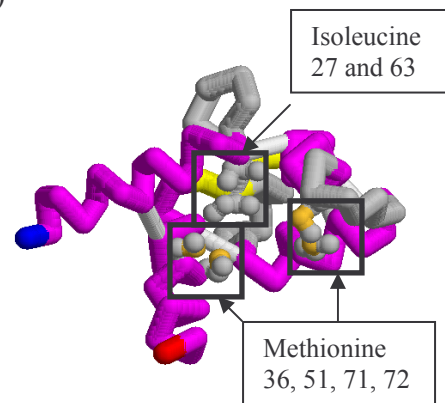
2 Isoleucine



Please refer to the model for correct orientation of the specific amino acid sidechains.

(0.5 pt for correct position and 0.5 pt for correct orientation)

- To receive these points, the 6 amino acids that have been provided must be positioned properly numerically (amino acid 2 should be in the 2<sup>nd</sup> position), as well as 3-dimensionally (if the amino acid faces inward, then the foam sidechain should also face inward). If an amino acid is positioned correctly numerically, but faces the wrong direction, the model should receive 0.5 pts.
  - The methionine amino acids should be placed at positions 36, 51, 71 and 72.
  - The isoleucine amino acids should be placed at positions 27 and 63.



10. Model is globular/compact (3-dimensional)

- To receive these points, the model should be 3-dimensional (not flat and 2-dimensional). Proteins are 3-dimensional in shape and yet oftentimes students will fold their model in a 2-dimensional fashion so that the model is flat. Therefore, to receive these points, the model should be globular.
- This model should be compact in that the structural features are not too far apart creating a very large space between any one feature.

11. The amino and carboxy termini are positioned on the same side of the protein.

- To receive this 0.5 points, the model should have both N- and C- termini located on the same side. If you position the model as is shown in the figure to the right, please note that the N and C termini are on the same side (to the right of the line down the center).

