

Guide to Using the Rubric to score the Calmodulin Pre-build Model for Science Olympiad State 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 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 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

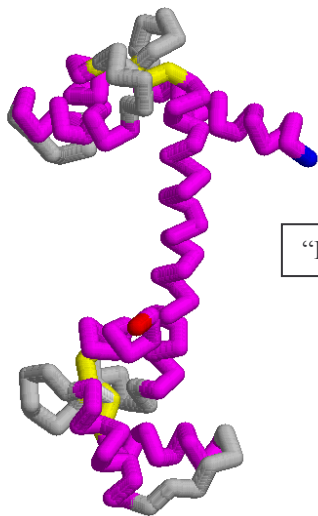
Color Code

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

N-terminus calcium binding domain

Central Helix

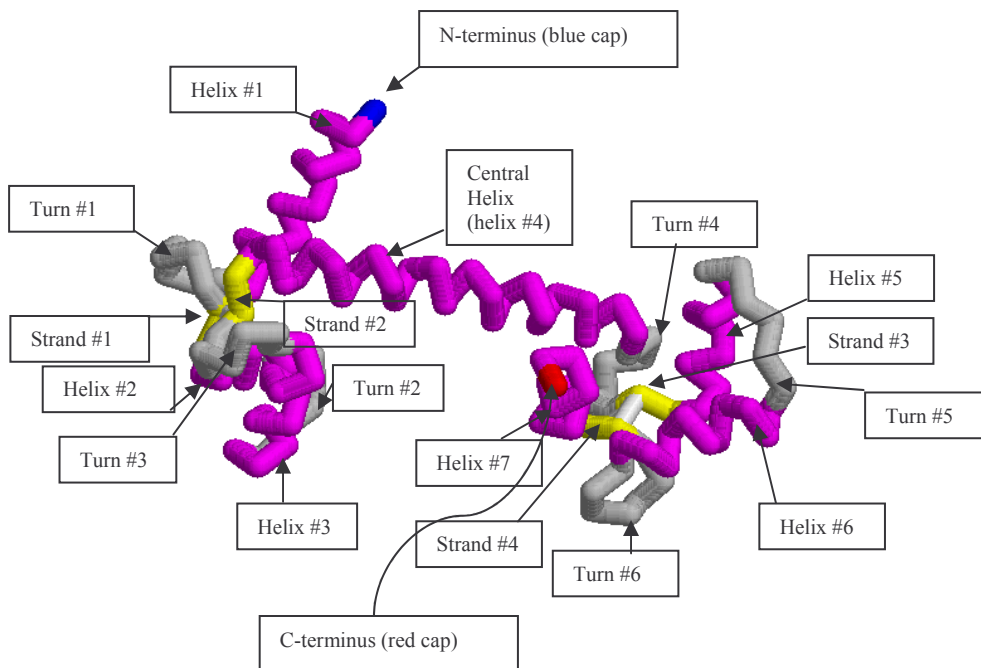
C-terminus calcium binding domain



“Dumbbell” shaped protein

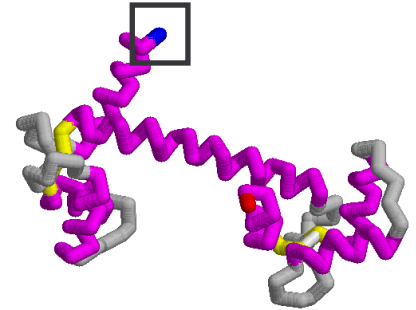
Order of structures:

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



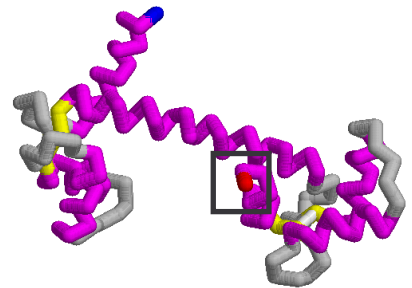
1. Blue Cap on N-terminal Amino Acid (Leu4)

- To receive one point, 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.
- Please note that the N-terminal helix is longer than the C-terminal helix, and the N-terminal helix leads into a turn, which the C-terminal helix is preceded by a β -strand.



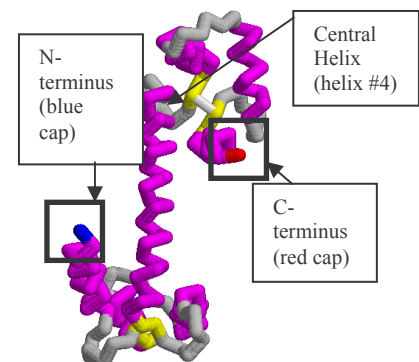
2. Red cap on C-terminal Amino Acid (Ala147)

- To receive one point, 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.
- Please note that the C-terminal helix is shorter than the N-terminal helix and that a β -strand precedes this helix whereas the N-terminal helix leads into a turn.



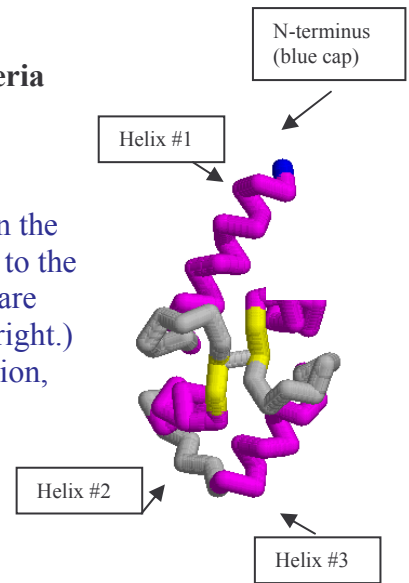
3. N and C termini are located on opposite sides of the axis of the central helix.

- 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.

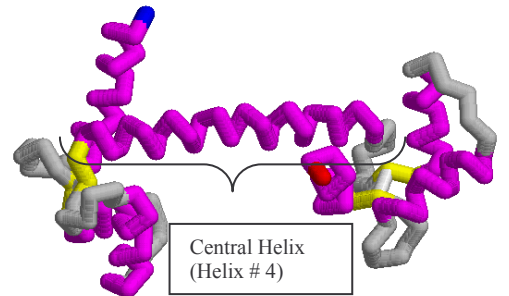


4. Model has 7 alpha helices according to Jmol/RasMol selection criteria

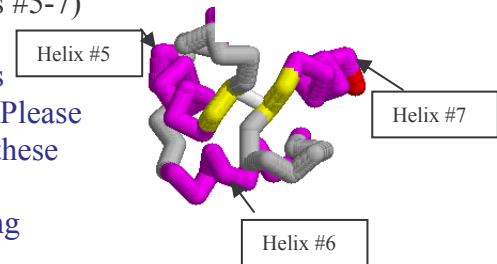
- 3 helices in N-terminus calcium binding domain (helices #1-3)
 - To receive these points, there should be 3 helices within the N-terminus calcium binding domain. Please see figure to the right for the correct location of these helices. (Helices are colored magenta on the model and on the figure to 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 the correct length and have appropriate number of amino acids/turn (~3.6 amino acids/turn)

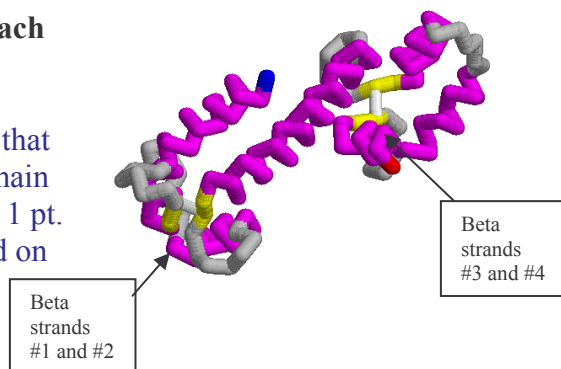
- To receive these points, each helix should be the correct length. For each correctly modeled helix, 0.5 pt should be awarded, for a total of 3.5 points.
 - Helix #1 is 16 amino acids long (Amino acids 4-19) (~4.5 turns)
 - Helix #2 is 9 amino acids long (Amino acids 29-37) (~2.5 turns)
 - Helix #3 is 11 amino acids long (Amino acids 45-55) (~3 turns)
 - Helix #4 is 28 amino acids long (Amino acids 65-92) (~7.5 turns) – this central helix should by far be the longest helix in the model
 - Helix #5 is 10 amino acids long (Amino acids 102-111) (~2.8 turns)
 - Helix #6 is 11 amino acids long (Amino acids 118-128) (~3 turns)
 - Helix #7 is 10 amino acids long (Amino acids 138-147) (~2.8 turns)
- To receive the 0.5 pts per helix, each helix should be roughly equivalent to the lengths described above. If the helix is 2 turns rather than 2.5 turns, then the helix should still receive the 0.5 pt. If the helix is 4 turns and only supposed to be 2 turns, then the helix is too long and should not receive the 0.5 pt.
- Please use the physical (z-corp plaster) model to help further in determining the length of the helices on the toober model.

6. 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 0.5 point, for a total of 3.5 points if all seven helices (Helix #1-7) are correct. It is not uncommon to have a model with a mixture of right and left-handed helices, so please take the time to check each helix.
- 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 put your right hand on the toober as if you were going up the toober 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.

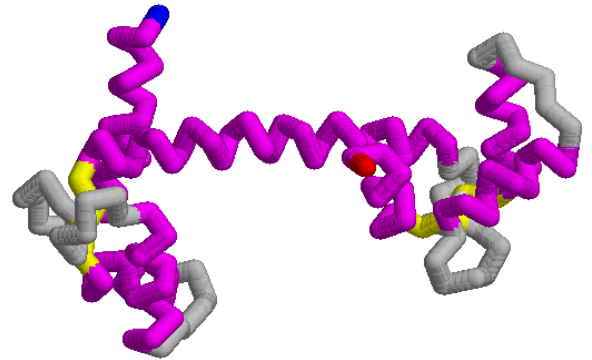
7. Model has one beta sheet (comprised of 2 strands) on each calcium binding domain

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



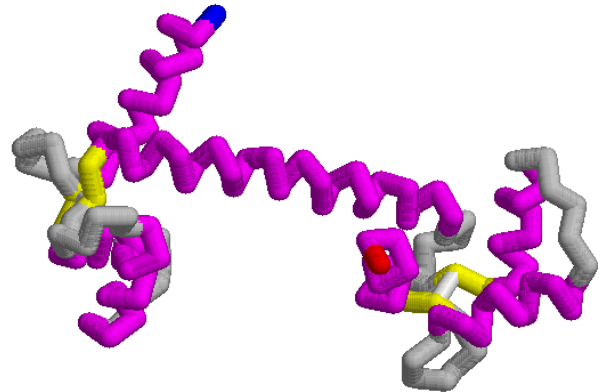
8. Model is dumbbell-shaped (one binding domain on either side of the central helix)

- 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).



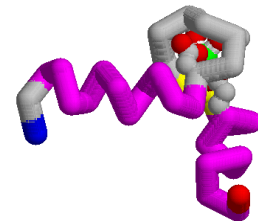
9. Positioning of secondary structures in the proper order

- 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



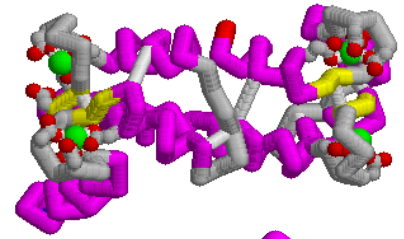
10. Model has 4 Helix-Turn-Helix Calcium Binding Groups (EF-Domains)

- An EF-Domain is a helix-turn-helix region or motif within the protein. The EF domain will begin with a helix and end with a helix. The two helices are separated by a turn region. The two helices are roughly perpendicular to one another, as seen on the figure to the right.
- There are 4 of these domains within the calmodulin protein – two on each side of the central helix. Each domain found within the model should receive 1 pt.

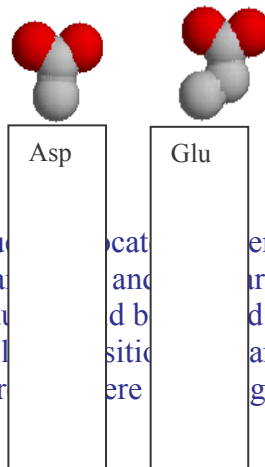
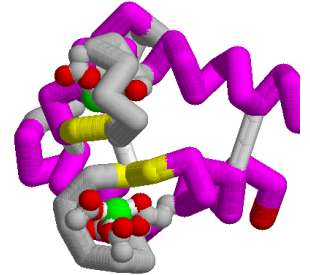


11. Creative additions to the model

- 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.

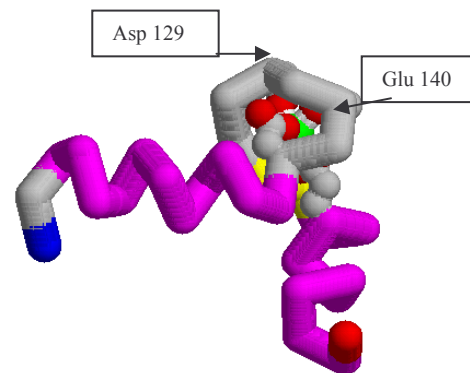
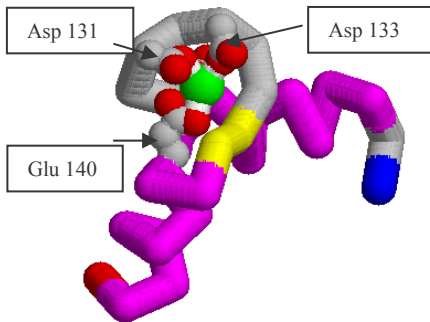


- Amino acids involved in coordinating the calcium ions are displayed (3 Aspartic acid amino acids and 1 glutamic acid amino acid per calcium ion). Oxygen atoms of the amino acids should be facing the calcium ion binding pocket, rather than out away from the model.

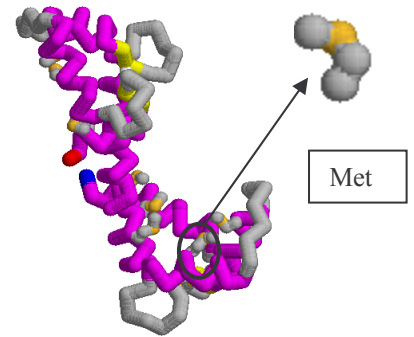


- The aspartate residues coordinate every other amino acid position (For example, 129, 131 and 133 are positioned on the loop region. The glutamate residues are positioned farther from the aspartate residues (for example, 140 is positioned on the helix. The glutamate is the only one to be positioned here and the model represents the calcium.

For example, shown below is one calcium binding domain:



- 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.
 - The additions must be accurate and reasonable.
 - Additions must be described and justified.

***Please note – if a model has all of the amino acids included on it, this feature does not tell the story of calmodulin. Therefore, accuracy points will not be awarded. Please see below.

12. Creative additions are important to functional importance

- To receive these points, the creative additions need to be relevant to telling the functional story of the protein. These points should not be awarded to models that have displayed all of the amino acids. The focus of adding the amino acids should be on the ones that play a role in the function of the protein. The focus of this protein is binding calcium and binding to the target proteins. Therefore, it is relevant to highlight these amino acids.

13. Creative additions are accurate

- To receive these points, the creative additions need to be accurate – in other words, the model cannot have the amino acids or other additions in inappropriate places. The additions need to reflect the scientific information that has been provided either in Goodsell's Molecule of the Month, the PDB file, or alternative resources.

14. 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. If the card does not adequately describe the creative additions, these points should not be awarded. At no time should the scorer have to guess what the team was trying to convey with their additions.