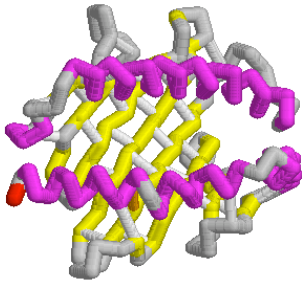
Guide to Using the Rubric to score the MHC Model

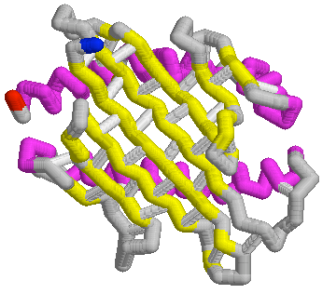
These instructions are to help the event supervisor and scoring judges use the rubric developed by the Center for BioMolecular Modeling in scoring the Science Olympiad Regional 2007 models of MHC, based on 1HSA.pdb. Each category on the rubric is addressed within these instructions and is accompanied by a short description and picture, if appropriate.

Overview of the model

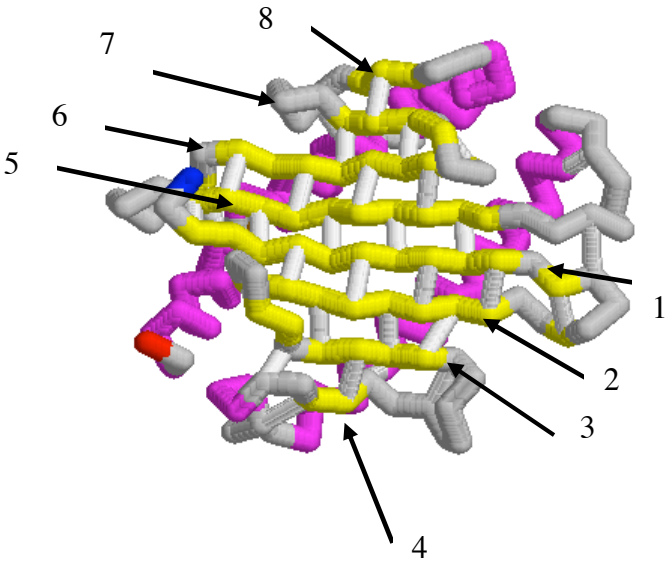
MHC Model looking down at the helices



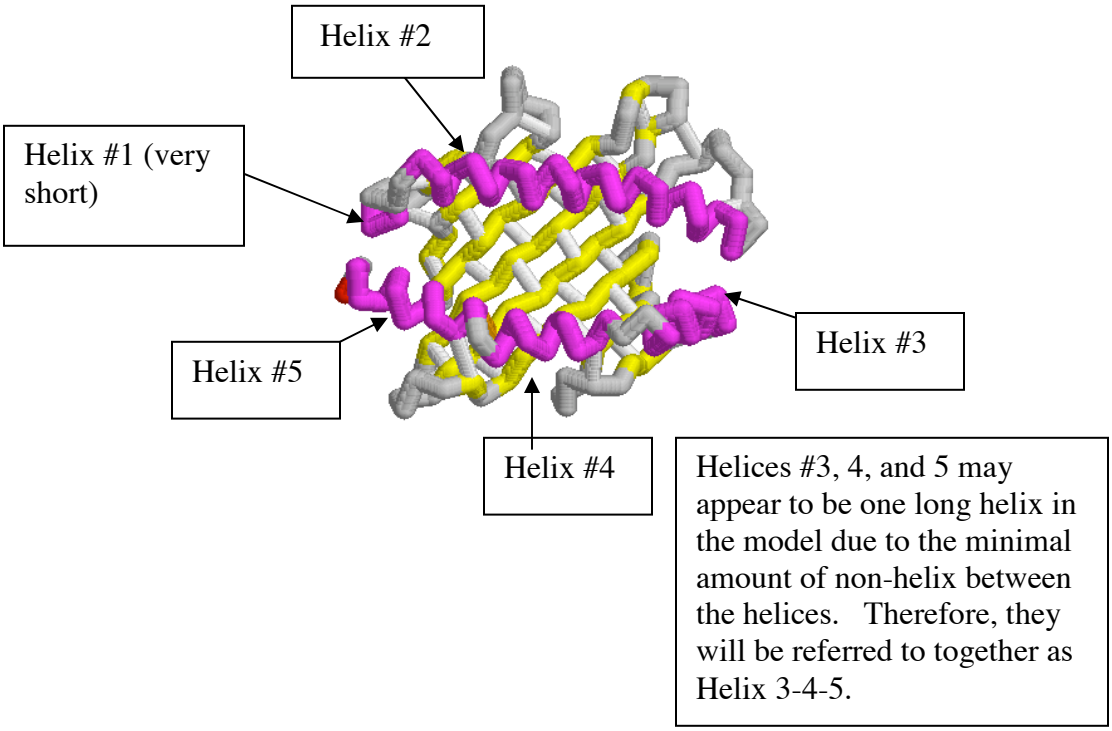
MHC Model looking at the sheets



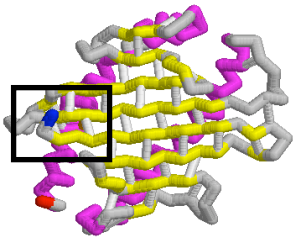
Numbering of the beta strands
This is how the beta strands will be referred to in the course of the rubric and guide to understanding the rubric.



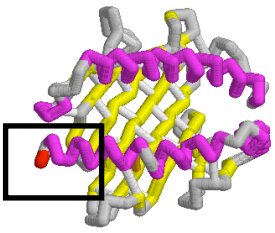
Alpha Helices
This is how the alpha helices will be referred to in the rubric and the guide to the rubric.



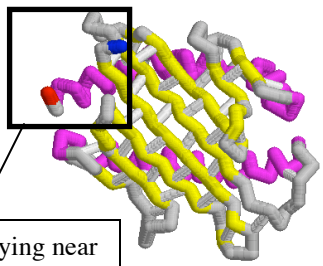
1. Blue Cap on N-terminal Amino Acid (Gly1) (1 pt)
   - To receive one point, the blue cap needs to be located at the N-terminus of the protein, which is the middle strand of the beta sheet. Please see the figure to the right for the correct positioning of the end caps.



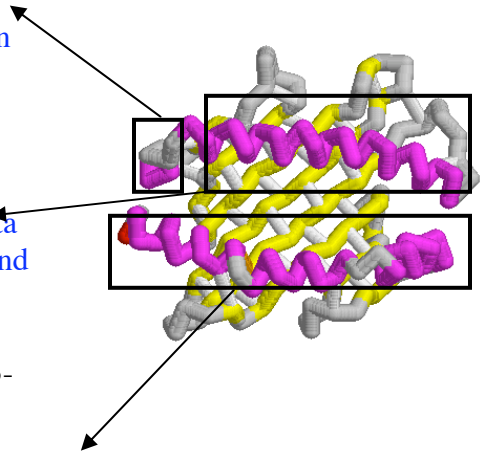
2. Red cap on C-terminal Amino Acid (Lys176) (1 pt)
   - To receive one point, the red cap needs to be located at the C-terminus of the protein, which is the end of the long helix. Please see the figure to the right for correct positioning of the end caps.



3. N and C termini are on the same side of the model, next to each other (1 pt)
   - To receive one point, the blue cap needs to be located near the red cap. Please see the figure to the right for positioning of the caps.

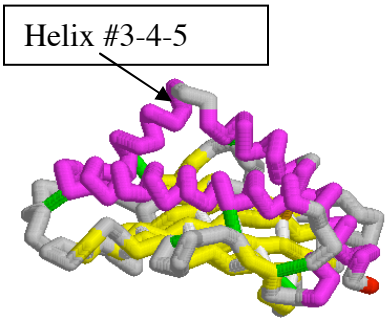


4. Model has 5 alpha helices according to RasMol selection criteria
    - A short helix (helix #1) after beta strand #4 and before the long helix #2 (1 pt)
        - To receive this point, there should be a short helix located between strand #4 of the beta sheet and the long helix #2 crossing the sheets. Please see figure to the right for the correct location of this helix.
    - One long helix (helix #2), which is located between the 4th and 5th beta strands (1 pt)
        - To receive this point, there should be a long helix, spanning the width of the beta sheet, and connecting strand #4 and strand #5 of the beta sheet together.
    - Three short helices (helices #3, #4, and #5), but will most likely appear as 1 long helix (helix #3-4-5) (1 pt)
        - To receive this point, there should be a long helix following the strand #8 of the beta sheet. The last part of the model is this helix. RasMol indicates that this section is actually made of 3 helices, but this may be hard to do with the toober, as there are only 1-2 amino acids between the 3 helices. Therefore, we refer to these as "helix #3-4-5". No point deductions for having 1 long helix, rather than 3.



5. Long helix (helix #3-4-5; at the C-terminus) should be longer than the helix #2 (1 pt)
    - To receive this point, the helix at the C-terminus (helix #3-4-5) should be longer than helix #2.

6. The longest helix (helix #3-4-5) should be bent upward, rather than straight, like that which should be seen with the helix #2 (1 pt)
    - To receive this point, helix #3-4-5 (longest one) should be positioned in such a way that there is more space between the beta sheets and the helix then there is between helix #2 and the sheet. Please refer to the picture to the right for further information.



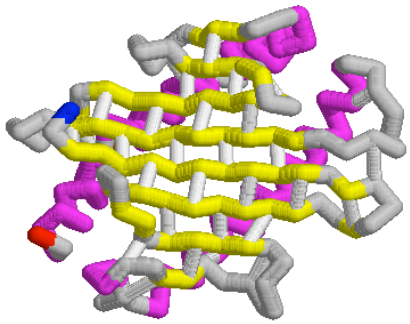
7. Alpha helices are right-handed (0.5 pt each; total of 1.5 pts)
    - Alpha helices are right-handed. Check each alpha helix in the model to confirm that the helix is right-handed. For each right-handed helix, the model should receive 0.5 points, for

a total of 1.5 points if all three helices (Helix #1, Helix #2 and Helix #3-4-5) 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, your have a right-handed helix. If you would put your left hand on the toober, you have a left-handed helix and the model would not receive the points.

8. Model has 1 section of beta sheets with 8 strands (0.25 pt per strand; for a total of 2 pts)

- To receive these points, there should be 8 strands that make up the beta sheet section of the model. Each strand present is worth 0.5 pt.

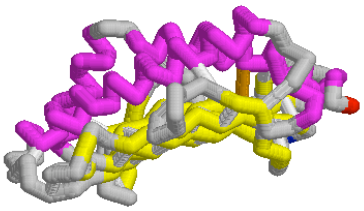


9. Beta sheet is an anti-parallel sheet (1 pt)

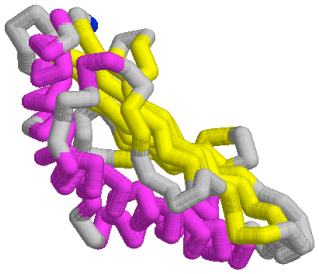
- To receive this point, the strands of the beta sheet should be anti-parallel.
- One strand should be running N-C and then one lying next to it will be C-N.
- This would translate in a back and forth fashion (one beta strand leading into another one with a hairpin loop separating them).

10. Model is compact, in that the alpha helices are not very far away from the beta sheets (1 pt)

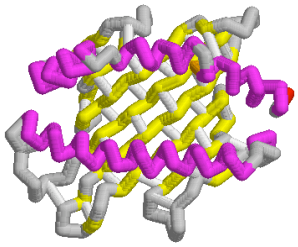
- To receive this point, the model should have a compact look to it – the alpha helices should not be more than 2 inches above the beta sheet at the highest point (2.5 inches is okay, 3 is not).
- There should also be space between the beta sheets and helices, so if the helices are lying right on the beta sheets, the model should not get this point. Essentially, when you look at the model from the side, it should have two layers – one of which has the two alpha helices and one of which has the beta sheets.



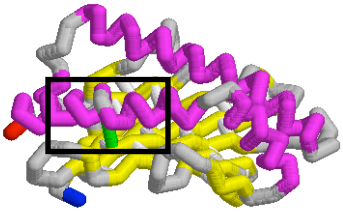
11. Beta strands are in the same plane with one another (1 pt)
    - To receive this point, the beta strands should be lying next to one another in the same plane.
    - The beta strands should not be above or below each other in any significant way. Please refer to the figure on the right.



12. Helices cross the beta sheet (0.5 pt for each helix; 1 pt total)
    - To receive these points, the two long helices should cross the beta sheets.
    - The alpha helices are not parallel to the beta strands, but rather the helices are tilted about 45 degrees from the beta sheets.

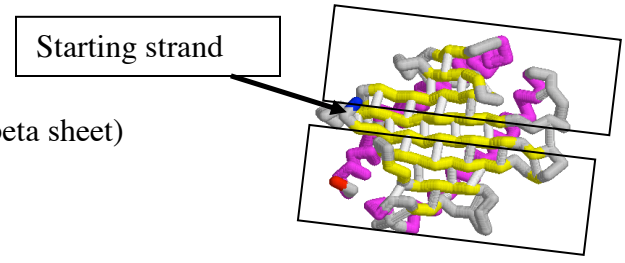


13. Disulfide bond connecting helix #3-4-5 (the longest one) to strand #5 of beta sheet (1 pt)
    - To receive this point, there should be a disulfide bond shown connecting helix #3-4-5 (the last helix/C-terminus) to strand #5 of the beta sheet.
    - The disulfide bond is in between Cys 101 and Cys 164 (the model is 176 aa long)



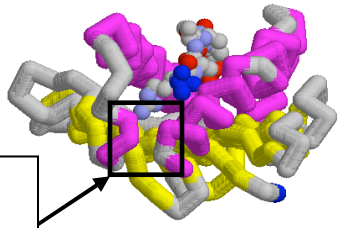
Disulfide bond (in green on this figure)

14. The sequence of model is correct: (2.5 pts)
    - N-terminus/beta strand #1-beta strand #2
    - Beta strand #2-beta strand #3
    - Beta strand #3-beta strand #4
    - Beta strand #4-alpha helix #1
    - Alpha helix #1-Alpha helix #2 (over beta sheet)
    - Alpha Helix #2 –beta strand #5
    - Beta strand #5-beta strand #6
    - Beta strand #6-beta strand #7
    - Beta strand #7-beta strand #8
    - Beta strand #8-Alpha helix #3-4-5(over the beta sheet) – C terminus

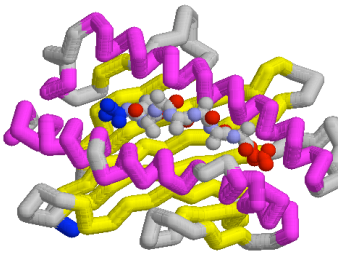


- To receive these points, the model must follow this sequence.
- Additionally, the model should have symmetry to it, as there are 4 strands, then a helix, then another 4 strands and a helix.

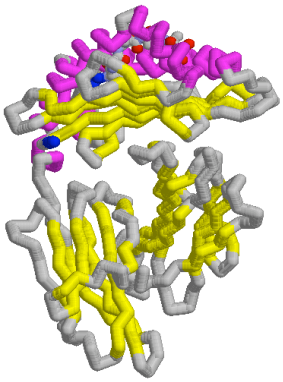
15. Creative additions to the model (6 pts)
    - Flu peptide piece laying between the two helices (please see figure on next page)
    - Flu peptide is 9 amino acids in length (all alanines, except for Arg at position 2)
    - Flu peptide is arranged so that the Arg is facing the beta sheet (serves as anchor point; please see picture to the right for positioning)



    - Flu peptide is oriented so that it is lying in the groove with the N-terminus facing the N-terminus of the protein (please see figure to the right for orientation; blue amino acid in peptide is the first amino acid, red amino acids in pepetide is the last amino acid of the peptide)



    - Other portions of the model (they are required to only model the first 176 amino acids), there are 276 amino acids in chain A, and 99 amino acids in chain B



    - 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 the MOM.
        - Additional features that are explained (in the abstract or labeled on the model) that help to tell the story are also okay.