

Guide to Using the Rubric to score the Insulin 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 Insulin, based on 2HIU. Each category on the rubric is addressed within these instructions and is accompanied by a short description and picture, if appropriate.

1. Blue cap on N-terminal amino acid of chain A (shorter chain; N-terminus is pale blue on model)

- To receive one point, the blue cap must be positioned correctly on chain A. Please see the figure to the right for the correct positioning of the end caps.

2. Blue cap on N-terminal amino acid of chain B (longer chain; N-terminus is dark blue on model)

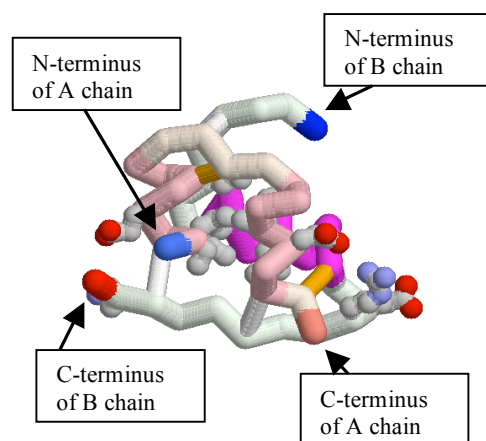
- To receive one point, the blue cap must be positioned correctly on chain B. Please see the figure to the right for the correct positioning of the end caps.

3. Red cap on C-terminal amino acid of chain A (shorter chain; C-terminus is pale red on model)

- To receive one point, the red cap must be positioned correctly on chain A. Please see the figure to the right for the correct positioning of the end caps.

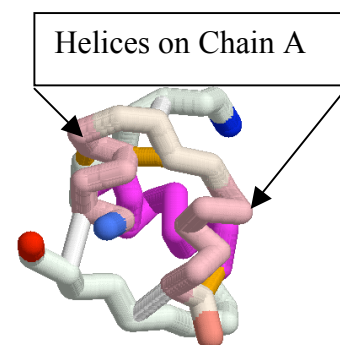
4. Red cap on C-terminal amino acid of chain B (longer chain; C-terminus is dark red on model)

- To receive one point, the red cap must be positioned correctly on chain B. Please see the figure to the right for the correct positioning of the end caps.



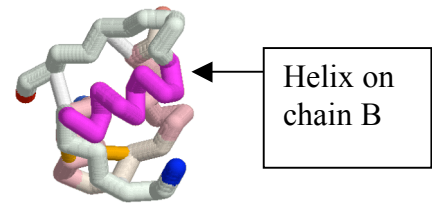
5. 2 Alpha-helices on chain A (shorter chain; pink on model)

- Chain A is the shorter of the two chains. There should be two helices on this chain. The model has these two helices colored pink.



6. 1 Alpha-helix on chain B
(longer chain; magenta on model)

- Chain B is the longer of the two chains. To receive two points, there should only be one helix on this chain. This helix is colored magenta on the model.

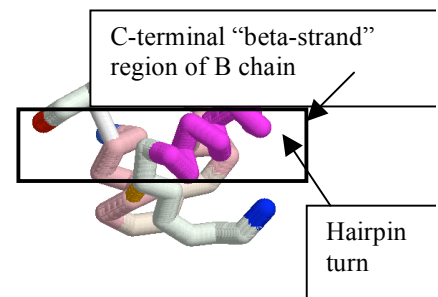


7. Alpha helices are right-handed

- 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 points, for a total of 1.5 points if all three helices 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, you 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.

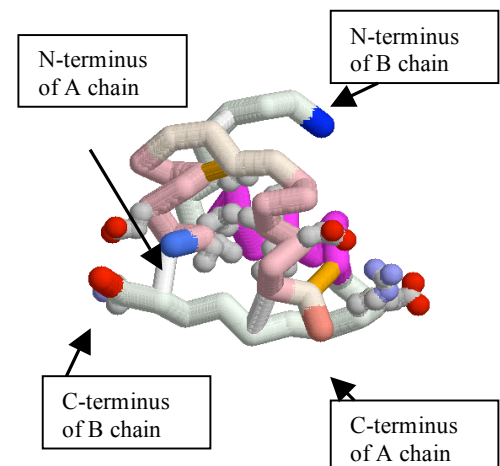
8. The C-terminus of the B chain (longer chain) is at the end of a section that resembles a beta-strand and this “beta-strand” is located close to the beginning of alpha helix within this chain

- To receive 0.5 point, the toober model should have a region at the C-terminus of the B chain that is straight, or bent like a paper fan, to resemble something similar to a beta-strand.
- To receive the remaining 0.5 point, this beta-strand region should be positioned so that it is bent back toward the alpha helix of the B chain (magenta). At the end of the helix, there should be a hair pin loop that allows this terminal portion of the protein to be bent back in the same direction as the helix.

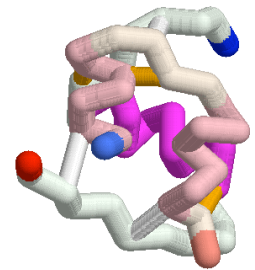


9. Chain A is correctly positioned in relation to chain B The alpha helices of chain A are nearly parallel.

- Chain A alpha helices are in pink on the model.
- The N and C termini of chain A are pointing in the same direction.
 - The A chain is the shorter chain and on the model is designated by the chain with the pink helices and the N and C termini are designated by the lighter colors. If you trace the path of chain A, there should be a hairpin separating the two helices, so that they run in opposite directions. The N and C termini of Chain A should be pointing in the same direction (rather than one pointing upward and one pointing downward).



- Both N and C termini of chain A are positioned close to the C-terminus of chain B
 - The A chain is the shorter chain and on the model is designated by the chain with the pink helices and the N and C termini are designated by the lighter colors. The B chain B-sheet is white in the model, and is terminated by the red C-terminal end cap. The two ends of the A chain should be lying near the B-sheet of the B chain.
- The N terminus of chain A lies near the C terminus of chain B
 - The N and C termini of chain A should be positioned so that they are near the C-terminal region of the B chain, rather than the N terminus of the B chain. In order to receive the 0.5 points, the N-terminus of the A chain (light blue) should be the terminus closest to the C-terminus of the B chain. The C-terminus (light red cap) of the A chain should be further away from the C-terminus (dark red cap) of the B chain. Please see the picture of the model above.
- The alpha helices of the A chain are in the same plane and lying next to each other.
 - Chain A has two alpha helices separated by a single “straight” region. So, the toober will resemble a “U” in which the stems of the “U” are helices. These helices are in the same plane as one another; they are not positioned to be above or below one another; if you took that chain off of the model, the helices should lie fairly flat next to each other. If the toober representing chain A illustrates this feature, give the model 0.5 point. (Please see figure to right; sidechains have been removed to simply the image. Chain A has the pink helices.)
- The helices are positioned perpendicular to the helix on the B chain.
 - The alpha helices in chain A should lie perpendicular over the alpha helix in chain B. Looking at the model with the two helices on the top, if you look beneath these two helices, there should be another helix lying underneath it. If the toober model has this feature, the model should receive another 0.5 point. (Please see figure to right; sidechains have been removed to simply the image. The pink helices are located on Chain A. The magenta helix is on Chain B.)
- There should be two “layers” to the protein
 - When looking at the model, there should be evidence of two layers to the protein, rather than everything in the same plane, or a 2-D protein.
- The composition of each layer should be correct.
 - The model can be divided into two layers in one of two ways. If the model clearly shows at least one of these two patterns, it is correct.
- Pattern A:
 - The first layer consists of Chain A and the N-terminus of Chain B.
 - Looking at the model, the first layer should have Chain A, which should be one color toober and the N-terminus of Chain B, which is a different color toober with a blue cap on it.
 - The second layer should consist of the alpha helix and the C-terminus of the B chain.
 - The other layer should be the C-terminus of the B chain and the alpha helix of the B chain. It should contain only one toober color, of the longer chain, and should have a red cap.



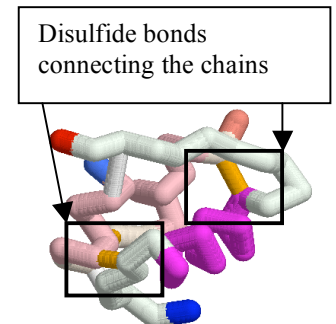
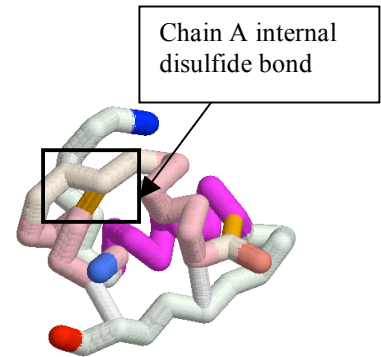
OR the model can have this pattern

- Pattern B:

- The first layer consists of Chain A and the C-terminus of Chain B.
 - Looking at the model, the first layer should have Chain A, which should be one color toober and the C-terminus of Chain B, which is a different color toober with a red cap on it.
- The second layer should consist of the alpha helix and the N-terminus of the B chain.
 - The other layer should be the N-terminus of the B chain and the alpha helix of the B chain. It should contain only one toober color, of the longer chain, and should have a blue cap.

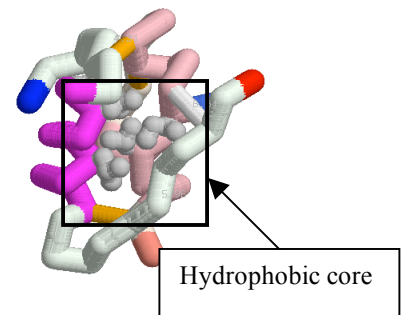
10. 3 Disulfide bonds are present in model and correctly positioned

- This model should have 3 disulfide bonds indicated. Each bond is worth one point. These disulfide bonds are essential to the overall structure of the model and hence should be designated. The materials provided did not include any materials that were meant to be used specifically as disulfide bonds, so the students should have been creative to indicate these special bonds. For instance, they may have taken the cross-linkers provided within the kit and colored them to designate them to be disulfide bonds versus basic stability structures. In the plaster model, disulfide bonds are in orange.
- One of the disulfide bonds is located within chain A, between Cys 6 and Cys 11
- The other two disulfide bonds hold the two chains together: Cys 20 on Chain A connected to Cys 19 on Chain B; Cys 6 on Chain A connected to Cys 7 on Chain B.



11. Hydrophobic amino acids are in the “interior” and correctly positioned (Ile2, Leu6, Leu11, Leu15, Leu16)

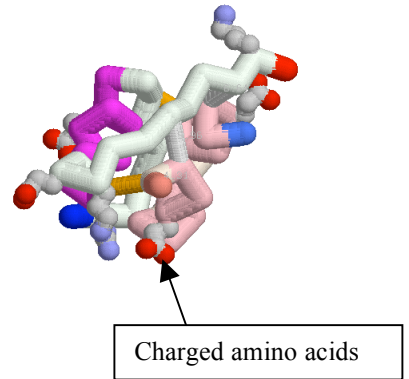
- The Molecule of Month article written by David Goodsell on the PDB describes a “hydrophobic core” that is composed of carbon-rich amino acids, such as leucine and isoleucine. As with the disulfide bonds, no materials were provided with the kits to indicate this feature, but this could be added to the model by the students in a number of different ways (previous students have chosen to model sidechains of amino acids with clay, paper clips, or paper cut-outs).
- 0.5 points should be given for inclusion of each of the amino acids listed above and if they are positioned correctly (so that these amino acids are facing inward and making a hydrophobic core). No hydrophobic amino acids should be located on the surface of the



model. On the picture to the right and on the scoring model, the amino acids that are gray represent the hydrophobic amino acids.

12. Charged amino acids are on the “surface” and correctly positioned (Glu4, Glu13, Glu21, Glu17, Arg22, Lys29)

- The Molecule of the Month article written by David Goodsell on the PDB describes the surface of the insulin protein as covered with charged amino acids, such as Lysine, Arginine and Glutamate. As with the disulfide bonds, no materials were provided with the kits to indicate this feature, but this could be added to the model by the students in a number of different ways (previous students have chosen to model sidechains of amino acids with clay, paper clips, or paper cut-outs).
- 0.5 points should be given for inclusion of each of the amino acids listed above and if they are positioned correctly (so that these amino acids are all located on the surface of the protein). None should be located facing inward as part of the “hydrophobic core” described in number 11. On the picture to the right and on the scoring model, the charged amino acids are colored with CPK coloring (carbon is gray, nitrogen is blue and oxygen is red).



13. Creative additions to the model

- Any additions to the model beyond what is described above should be awarded up to 1 point, as long as the additions are accurate.