

Science Olympiad Protein Modeling Event

Guide to Scoring Zinc Finger Motif

Once you have folded the zinc finger motif (chain C, residues 4-31 of 1ZAA.pdb), use this guide in conjunction with the rubric to evaluate the quality of your model. Although the features vary from model to model, the rubric and rubric guide emphasize the same characteristics that are evaluated in pre-build and onsite build models in Science Olympiad competitions. For further explanation of certain features, marked with an asterisk (*), see the Additional Scoring Guidelines.

Note on Scoring: As you work through this guide, it may be helpful to use both the scoring model and the images. You can quickly orient the model with the images by lining up the blue and red ends. There is also a quick reference scoresheet you may wish to use once you've become familiar with the structure

Topology and primary structure

1. **Secondary structures (helices, sheets, loops and turns) are in the correct order from N to C terminus (correct topology).**

Color Code:

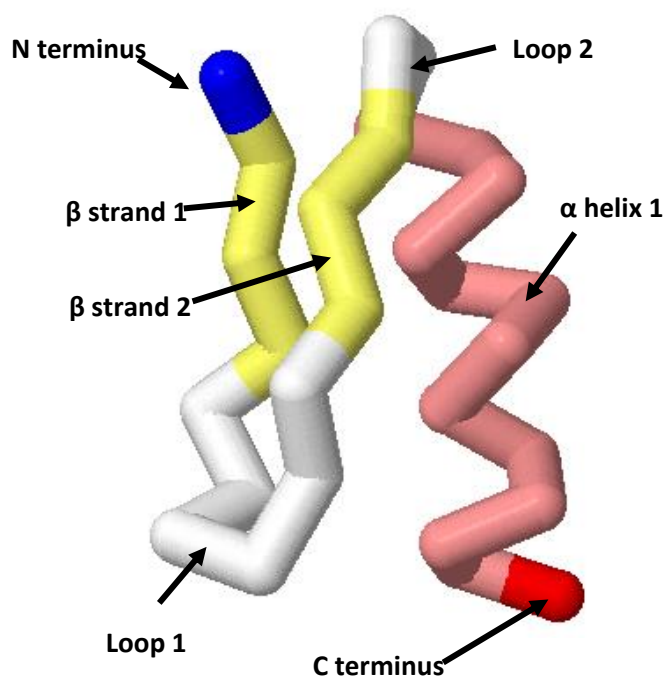
Salmon – alpha (α) helices

Yellow – beta (β) strands

White - loops

Blue tip – N-terminus

Red tip – C-terminus



The order of secondary structures is:

N terminus
 β strand 1
loop 1
 β strand 2
loop 2
 α helix 1
C terminus

Award 1 point for each secondary structural element (in bold) that is in the correct order. (5 points)

If two elements are reversed, deduct 2 pt.

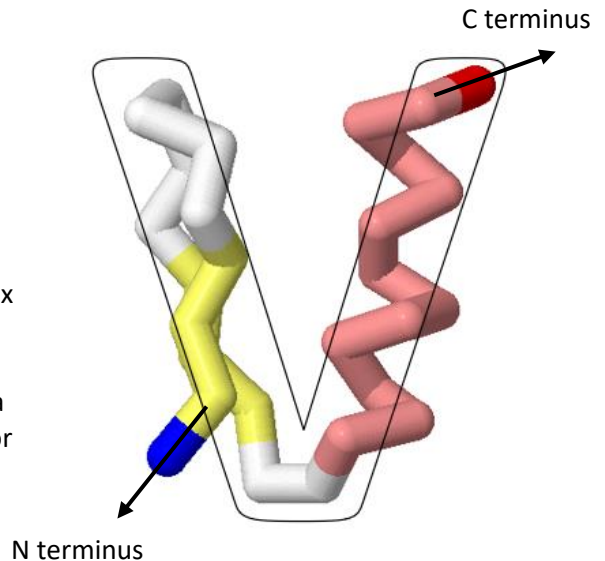
If a single element is missing, deduct 1 pt.

Secondary structures that are out of order should not be counted.

For parts 2 and 3, orient the model so that it is in the shape of a V, with the alpha helix on the right side.

2. N and C termini are identified correctly

- a. The blue endcap must be on the N terminus, adjacent to β strand 1. (0.5 point) If the blue endcap is next to a helix or loop, no credit is awarded.
- b. The red endcap must be on the C terminus, adjacent to a helix. (0.5 point) If the red endcap is next to a β strand or loop, no credit is awarded.



3. N and C termini are positioned correctly in the overall fold of the protein.

- a. The N terminus should be in front, at the base of the V, and pointing downward at approximately “7 o’clock”. (0.5 point)
- b. The C terminus should be on the top of the V, pointing upward at approximately “2 o’clock”. (0.5 point)

4. Model is at a scale of 2 cm per residue

Although it is difficult to assess whether the model is built to the appropriate scale, addressing the following two questions will allow you to reach a reasonable assessment.

- a. Is the model proportional – that is, the length of the two sides of the V are approximately the same? (0.5 point)
- b. Compare the model with the *group* of models being evaluated. Does the model take up approximately the same space as the *average* of all the model sizes? (0.5 point)

Secondary structure

5. Alpha helices

- a. The model has one helix. (0.5 point)
- b. The helix has 3-4 turns. (1 point) If the model has fewer than 3 or more than 4 turns, there is no credit.
- c. The helix is right handed.* (1 point)
- d. The helix is uniform in diameter.* (0.5 point)
- e. The coils in the helix are evenly spaced.* (0.5 point)

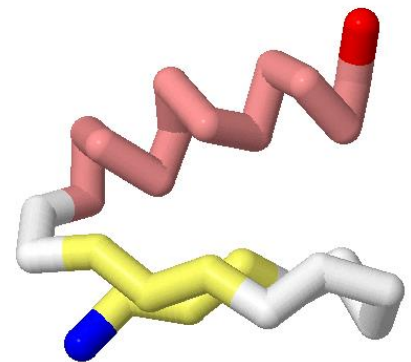
6. Beta sheets

- Beta strands are identified differently than loops. (Distinction may be color-coding, or clips at start and finish, or zig-zag bending of the beta strands, or any other way of marking sheets vs. strands.)* (1 point)
- There are two beta strands. (1 point)
- The two beta strands form a single beta sheet. (0.5 point)
- The two beta strands are approximately half the length of the alpha helix. (0.5 point)
- The two beta strands lie parallel to each other. (1 point)
- The two beta strands are antiparallel.* (0.5 point)
- The two strands of the beta sheet form a flat plane.* (It is not twisted.) (1 point)

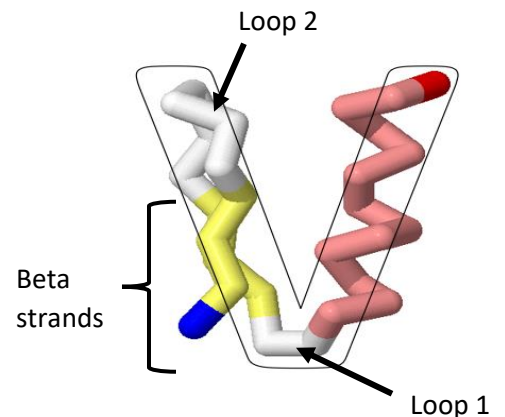
Tertiary structure

7. Secondary structures are oriented in three-dimensional space relative to each other

- Alpha helices are positioned correctly.** Place the model on the table with the two beta strands resting on the table. (See figure at right.) The helix should lie on top of the beta sheet base. (0.5 point)
- Alpha helices are oriented correctly.** The C terminus of the molecule should be the highest point of the model. (0.5 point)
- Beta sheets are positioned correctly.** When the model is oriented in a V shape, with the alpha helix on the right, the two beta strands should form the lower portion of the left side of the V. (0.5 point)

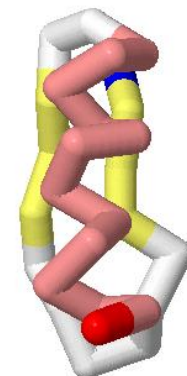


When the model is oriented with the alpha helix in front and the beta sheet in the back, the alpha helix should be framed between the two beta strands. The two beta strands should not be much wider than the helix. See image to left. (1 point)



- Beta sheets are oriented correctly.** With the V orientation (as above), the beta strand with the N terminus (beta strand 1) should lie in front of the second beta strand. (0.5 point)
- Loops are properly positioned in the model.** In the V orientation, loop 1 should form the base of the V. (0.5 point)

In the V orientation, loop 2 should form the upper half of the left side of the V. (0.5 point)



8. Overall shape of protein matches that of the pdb structure

The folded structure of the zinc finger motif should resemble a V, with the helix forming one side of the V and the beta sheet forming the other side of the V. If the model does not have a V shape, no credit is awarded. (1 point)

9. Spacing of structures is even and aesthetically pleasing

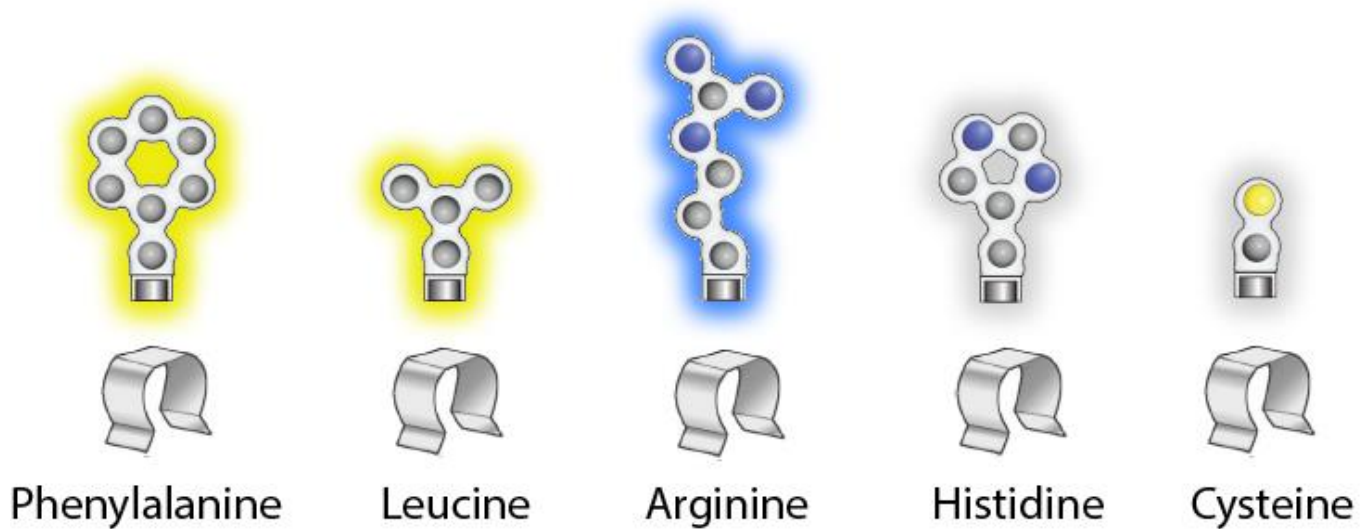
The two sides of the V should be of equal length. (1 point)

The angle between the helix and sheet should form a V. (1 point) If the model looks more like an I or an L no credit is awarded.

Specific sidechains (On-site build only)

Typically, only a few sidechains are included in the onsite build. The Zinc Finger Folding Activity includes 7 sidechains. Descriptions for position and orientation of all sidechains is provided here, but only a subset of sidechains is scored.

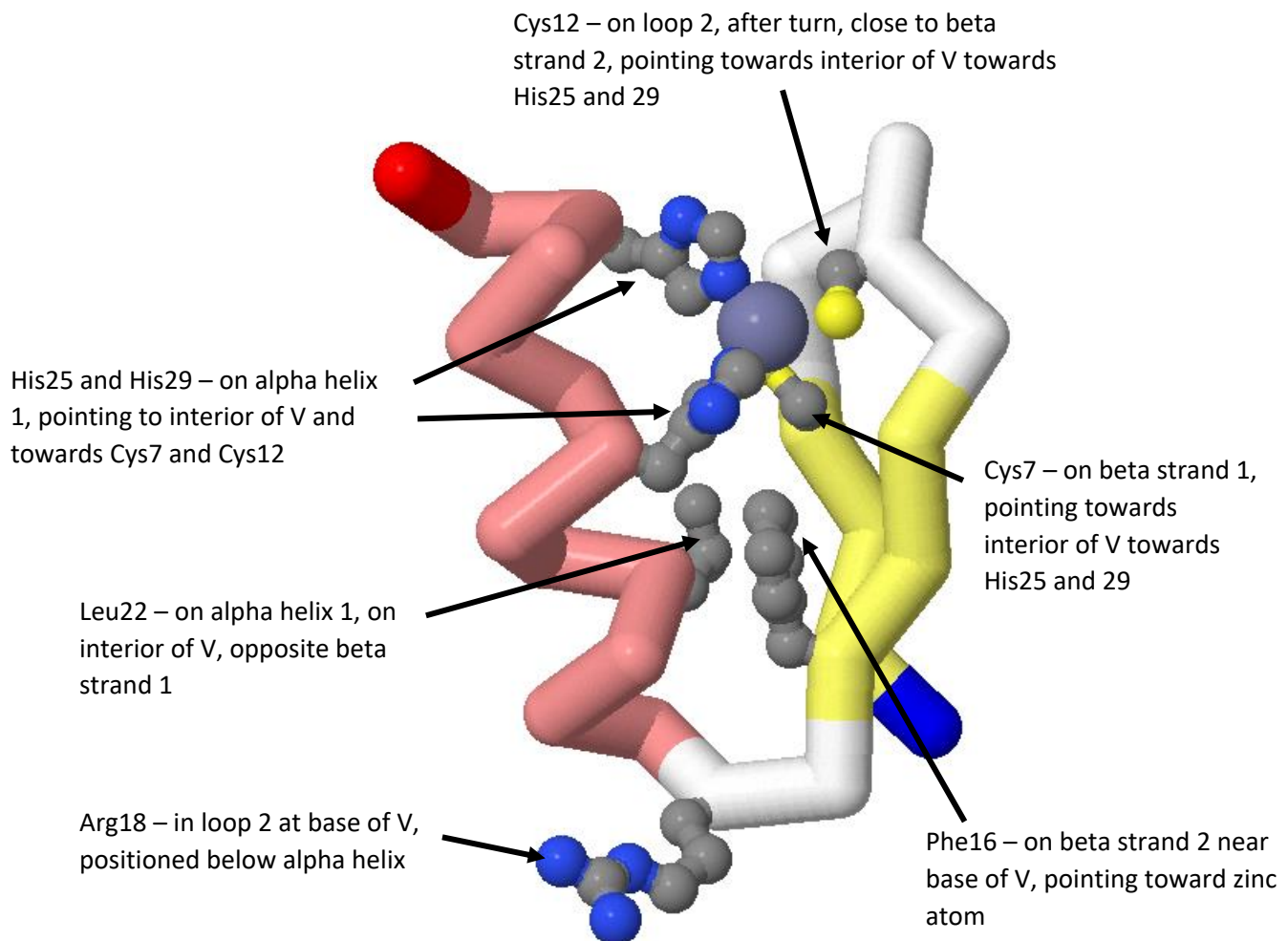
Sidechains and their identity:



10. Designated sidechains are positioned correctly on the alpha carbon backbone

11. Designated sidechains are oriented correctly (facing in the same direction as the pdb structure).

Sidechain	Position	orientation
Cys7	On beta strand 1, approximately midway up the "V". (0.5 point)	These four residues face towards each other on the interior of the model (inside the V). All four residues should be positioned to interact with the zinc atom. (2 points)
Cys12	On loop 1, after the bend and in line with beta strand 2. (0.5 point)	
His25	On alpha helix 1, midway up the "V". (0.5 point)	
His29	On alpha helix 1, near the top of the "V" (close to C terminus). (0.5 point)	
Phe16	On beta strand 2, near base of "V".	On interior of V, pointing towards the top of the V.
Arg18	In loop 2 at base of V. (1 point)	On outside of V, positioned below the alpha helix. (1 point)
Leu22	On alpha helix, near base of "V".	Across from, and facing beta strand 1.



Additional features (Pre-build only)

This section lists additional parameters for the pre-build model. These are features that are added by the team to tell the molecular story of the protein structure-function. The Zinc Finger Folding Activity more closely resembles the on-site build.

10. Creative additions are

- a. Positioned correctly
- b. Described accurately
- c. Contribute to the molecular story of the protein

11. 4"x6" notecard is included

- a. Follows appropriate format (what, how, why table)
- b. Describes creative additions

12. Other design parameters

- a. Model fits within 2'x2'x2' space
- b. Model is sturdy enough that judges can pick it up for judging
- c. Model is accessible from all sides for judging
- d. Pre-build model and notecard are impounded prior to the start of the competition