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3.04 Exploring ATCase: superimposing

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Now for the fun part! Let's examine the structural changes that occur between the R-state and the T-state of ATCase.

1. Make sure that both the R-state and T-state are toggled on. It might be nice to color the regulatory and catalytic subunits of each state a different color for the best viewing.
2. Superimpose the two states using the "super" command. Note: these are large structures, so the superposition could take a little while. Be patient!

PYMOL: ATCase superimposing Q1

1/1 point (ungraded)

After you have superimposed the structures (using super), you should be able to see the RMS (root mean squared deviation) for the alignment.

As you learned in the last unit, the RMS is a measurement of how different the structures are. The higher the number, the greater the difference between the states.

What is the RMS between the T-state and the R-state?

6.242

✓

6.242

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You have used 2 of 2 attempts

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PYMOL: ATCase superimposing Q2

1/1 point (ungraded)

The overall ATCase conformational changes result in one state being more spherical and the other a bit less spherical, which is particularly prominent when comparing position of the two catalytic trimers. Which state is most spherical?

R-state

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PYMOL: ATCase superimposing Q3

3/3 points (ungraded)

This problem may be a challenge!

Let's figure out where the largest structural changes occur in individual subunits between the T state and the R state. We will answer this question: do the catalytic subunits change the most, or the regulatory subunits?

First, write selectors for the "H" (regulatory) chain of the T-state and R-state. Use super to superimpose these two chains. What is the RMS between these chains?

1.548

✓

1.548

Next, write selectors for the "A" (catalytic) chain of the T-state and R-state. Use super to superimpose these two chains. What is the RMS between these chains?

0.977

✓

0.977

Which subunit shows larger conformational changes?

☐ Chain A (catalytic)

☒ Chain H (regulatory)

✓

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You have used 2 of 2 attempts

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Here are some other things you can try:

- Superimpose using all regulatory chains
- Superimpose using all catalytic chains
- Superimpose using just a subset of chains (for example, A,B,C)

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