

3.02 Explore the R-state

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Now that the script is loaded, you should see two different proteins: ATCase in its T-state and its R-state.

If you do not see structures named "T-state" and "R-state," repeat the loading procedure shown on the previous page!

Below are a few questions to guide your exploration of the ATCase structures. You may want to save a scene (and save your session) after each question, which will make it easier to step back to previous questions or continue to navigate the structures on your own later.

Start with these exercises:

1. Toggle the T-state off, so you only see the R-state
2. Show the structure as cartoons. Remember, you do this by clicking on the "S" menu on the right, and selecting show → as → cartoon
3. Color the subunits by chain. Remember, you do this by clicking on the "C" menu on the right, and selecting color → by chain. We recommend that you use the first color scheme option, it will recolor only the carbon atoms and maintain conventional coloring of other atoms like oxygen and nitrogen.
4. Select the PALA bisubstrate analog: type "select substrate, resn PAL" in the command line. You will see a new object, called substrate, that appears in the right hand menu.
5. Show the substrate as spheres, and make the substrate a different color so you can visualize it.

PYMOL: ATCase Explore the R State Q1

1/1 point (ungraded)

Now, make a new selection that ONLY selects the catalytic chains of the R-state of ATCase. Write a command that will just select these chains. When you have found a command that creates a new selection corresponding to only the catalytic chains, write that command below:

select catalytic, R-state AND chain A+B+C+D+E+F

✓

Submit

You have used 2 of 2 attempts

Show answer

PYMOL: ATCase Explore the R State Q2

1/1 point (ungraded)

If you were not able to select the catalytic chains of the R-state, do so now using the command above. Now, write a selection command for the **regulatory** subunits.

Color the catalytic and regulatory subunits two different colors (using the color menu or the command line). This might be a good time to save a scene, and then save your session!

Which of the options below best describes the arrangement of the structure of the regulatory and catalytic subunits of ATCase?

☐ Catalytic subunits are on the periphery of the structure, regulatory subunits are at the core

☒ Regulatory subunits are on the periphery of the structure, catalytic subunits are at the core

☐ Catalytic and regulatory subunits are mixed together in the structure

✓

Submit

You have used 2 of 2 attempts

Show answer

PYMOL: ATCase Explore the R State Q3

1/1 point (ungraded)

Now, write a selection that finds the residues that are near the substrate in the R-state. You may find the "around" command useful for this! The [PyMOL wiki selection algebra page](#) can be a useful resource.

Input the PyMOL selector string that you used here:

select active_site, byres (substrate around 6) and R-state

✓

Submit

You have used 2 of 2 attempts

Show answer

PYMOL: ATCase Explore the R State Q4

2/2 points (ungraded)

If you were not able to write a selector for the atoms near the substrate, use the answer to the problem above. Now, with the protein still shown as a cartoon, show the substrate as sticks, and color your active site selection a different color. (Hint: now could be another good time to save a scene!)

How many distinct active sites are there in the complete multimeric structure of R-state ATCase?

6

✓

6

Now, focus on the active site of chain B. You can either write a new selector, or find and zoom in on chain B. Color the substrate by atom. You may also want to label the atoms.

The substrate, PALA, contains a phosphate group. What structural feature is closest to the phosphate group of PALA on chain B of ATCase?

☐ A beta strand

☐ An alpha helix

☐ A long loop region

☐ A transition between a beta strand and a loop

☒ A transition between an alpha helix and a loop

✓

Submit

You have used 1 of 2 attempts

Save

Show answer

As you can see, there are many secondary structure elements close to the substrate of ATCase, many of which are loops.

This represents a common theme in enzyme active sites - they are often found in loop regions.

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