

3.01 Set-up

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Important Note: PyMOL work in this course is optional and ungraded! We cannot guarantee that PyMOL will work on your computer, and cannot provide Technical Support for PyMOL! Please work patiently and troubleshoot on your own!

To be prepared for this exercise, you need to complete the PyMOL exercises in unit 2 of this course.

You learned about the allosteric enzyme ATCase in the previous session. Remember, ATCase catalyzes the first **committed** step in the synthesis of pyrimidine bases. Even though its substrates (aspartate and carbamoyl phosphate) look nothing like a purine nucleotide, catalysis is allosterically regulated by the ultimate product of this pathway, cytidine triphosphate (CTP).

ATCase is considered a canonical allosteric enzyme for a number of reasons:

- It undergoes relatively large conformational changes between its T-state and its R-state (as you will see in this exercise!)
- It is subject to both homotropic and heterotropic allosteric regulation
- It is one of the best-characterized allosteric enzymes, functionally and structurally

In this exercise, you will explore ATCase in two different states:

- The R-state bound to the bisubstrate analog PALA, and
- The T-state bound to CTP.

PYMOL: Exploring ATCase Q1

3/3 points (ungraded)

Before we begin, test your knowledge with a few quick questions:

The T-state generally corresponds to the:

Inactive state



In the case of ATCase, the substrate aspartate is a:

☐ Negative homotropic allosteric regulator

☒ Positive homotropic allosteric regulator

☐ Negative heterotropic allosteric regulator

☐ Positive heterotropic allosteric regulator



In the structures you will explore, ATCase bound to the substrate analog PALA will be in the:

Active state



Submit

You have used 2 of 2 attempts

Show answer

PYMOL: Exploring ATCase Q2

1/2 points (ungraded)

To get started, look at the [PDB entry for ATCase bound to PALA \(the R-state\)](#).

How many regulatory subunits are there?

6



6

How many catalytic subunits are there?

5



5

Submit

You have used 2 of 2 attempts

Show answer

Now you are ready to start!

You are going to download a PyMOL script. This is a simple text file, which was written to automate the display of the full ATCase functional assembly based on the available crystal structures. Feel free to open the script in a text editor to find out more about the PyMOL commands used for that purpose.

Follow these directions carefully:

- Click [this link](#) to download a PyMOL script that will help you get started.
- Put the file in a folder of your choosing. For example, you might put it on the desktop.
- Open PyMOL and choose the "Run ..." option from the "File" menu. Navigate to the folder where you downloaded or saved the script. Select the script and click the "Open" button.
- You should see two structures load - named T-state and R-state.

Note: if the structures that load are not named "T-state" and "R-state", repeat the steps above, or try opening the ATCase loading script by double-clicking.

Reminder: It will be much easier to do this exercise with a 2 or 3-button mouse! It can be difficult to navigate PyMOL structures with a trackpad!

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