4.0.1 Exploring creatine kinase

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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.

Creatine kinase (CK) is a ubiquitous protein - functioning in different subcellular compartments, and even in different tissues. There are many different isoforms of the protein that have the same overall fold but minor structural differences. In this exercise, we will explore two isoforms - brain-type CK and mitochondrial-type CK.

First, explore the PDB documentation for three different structures of brain-type CK:

3DRB

3B6R

3DRE

Exploring creatine kinase: Q1

1/1 point (ungraded)

Look at the three different PDB entries, linked above. Look through the details of the structures. You'd like to start by exploring the active site of CK.

Which structure would be best for exploring the **active site** of creatine kinase?

- 3DRE
- 3B6R ✔
- 3DRB

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2/2 points (ungraded)

Although this series of exercises does not include regular reminders, please remember that it is good practice to save scenes and sessions regularly in PyMOL!

Open PyMOL and fetch the structure that is best for viewing the active site (see answer above if you need help!). Show the cartoon representation and find the ligands bound to the structure. One way to do this is by using the sequence view (Display → Sequence on) and selecting the ligands (you can just select them directly in the sequence view). Then represent them using sticks or spheres. You may also want to color the ligands a different color.

Note: In exploring this structure, we discovered that there is very low density in the area of the creatine, and the placement of the creatine does not make much chemical sense. The creatine is placed differently in the deposited PDB structure than in the published structure (see the paper here). As our knowledge progresses, this structure could become more refined!
Which subunit of CK is bound to the substrate analogs?

- Chain A
- Chain B ✔

What structural feature of CK is the closest to the amine group on the purine ring of ADP?

- A loop
- An alpha helix
- A parallel beta sheet
- An antiparallel beta sheet ✔

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Exploring creatine kinase: Q3

0/1 point (ungraded)

Ligand-protein hydrogen bonds can be mediated by water molecules. In this case the amine group of the purine ring is also hydrogen-bonded to a water molecule.

What 'residue number' is given to this water molecule?

601 ✖

601

Submit You have used 2 of 2 attempts Show answer

Exploring creatine kinase: Q4

0/1 point (ungraded)

What regions of CK would you expect to be the most evolutionarily conserved? Do you think the hydrophilic exterior of the protein would be well conserved? What about regions that interact with other subunits, what about the active site?

Write your answer below. Any answer is OK!

Yes ✖

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