

### 4.0.3 A structural view of conservation with ConSurf

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For the next section, we will use data generated from [ConSurf](#). To summarize, we provide ConSurf with a PDB entry, and we get back a new PDB file that has a new parameter - conservation score - for each amino acid in the protein.

ConSurf does this by performing a multiple sequence alignment of CK with other closely-related proteins, and then scoring the conservation of each amino acid in the protein based upon this alignment.

#### A structural view of conservation with ConSurf: Q1

2/2 points (ungraded)

When ConSurf generates a new PDB file, it overwrites the B-factor field of the file with "conservation scores." **B-factors** are a physical crystallography parameter.

Look through the ConSurf overview. For the "conservation score" parameter, what values represent **more conserved** amino acids?

☒ Lower numbers

☐ Higher numbers



Are conservation scores an absolute number, or a relative number?

☐ Absolute

☒ Relative



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We will be looking at the conservation of Brain-type CK (3B6R). Because the ConSurf server takes quite a long time to run, we have run 3B6R through this server for you. You can [click here to download the resulting PDB file](#).

Follow these steps carefully:

- Download and open the above-linked file in PyMOL.
- Change the background color to light grey. For example, you could use the command:  

```
bg_color grey80
```
- Show the whole protein as a ribbon.
- Write a selector for chain B. For example:  

```
select Brain_b, chain B
```
- Color the protein by B-factor (which is now conservation score.) Start with this command:  

```
spectrum b, blue_white_yellow, minimum=-1, maximum=1
```
- Show chain B as a cartoon.

You may also want to display the substrate, for example as spheres.

#### A structural view of conservation with ConSurf: Q2

1/1 point (ungraded)

If you have followed the above steps, you should see that chain A is colored all white, chain B is colored a spectrum between yellow and blue. Yellow represents **positive** conservation scores, while blue represents **negative** conservation scores.

Of the regions of chain B given below, which is the most conserved?

☐ The C-terminal loop

☐ The N-terminal alpha helix

☒ The only beta sheet in the protein

☐ The last alpha helix in the protein (going from the N-terminus to the C-terminus)



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#### A structural view of conservation with ConSurf: Q3

1/1 point (ungraded)

Why is the center of the protein more conserved? Do you think it relates to the active site, or the location relative to the hydrophobic core of the protein? Any answer is acceptable.

The hydrophobic core of proteins is often well conserved. This makes sense - a major change in even one residue (for example from hydrophobic to charged)

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#### A structural view of conservation with ConSurf: Q4

2/2 points (ungraded)

"ConSurf" is often used to represent the **surface** conservation of proteins! Show the protein as a surface. Be sure you can see the substrate bound in the active site (perhaps by showing it as spheres).

Is the substrate buried within the protein, or exposed on its surface?

buried

Look at the conservation of the residues around the substrate. Are they generally well conserved, or poorly conserved?

well conserved

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Bonus: compare the subunit interfaces of Brain and Mitochondrial-type CK.

You've already explored the conservation of Brain-type CK (3B6R). Just in case, you can [click here to download the resulting PDB file](#).

If you'd like, you can also download the ConSurf-generated PDB file for Mitochondrial-type CK: [click here to download the resulting PDB file](#).

For your reference, here are the steps again:

- Download and open the above-linked file in PyMOL.
- Change the background color to light grey. For example, you could use the command:  

```
bg_color grey80
```
- Show the whole protein as a ribbon.
- Write a selector for chain B. For example:  

```
select Brain_b, chain B
```
- Color the protein by B-factor (which is now conservation score.) Start with this command:  

```
spectrum b, blue_white_yellow, minimum=-1, maximum=1
```
- Show chain B as a *surface*.

You may also want to display the substrate, for example as spheres.

#### A structural view of conservation with ConSurf: Q5

0/1 point (ungraded)

For Mitochondrial-type CK, chain A has conservation scores saved in the B-factor field. By toggling the display of the different chains, you can explore the **interface** between the subunits of the dimer (for Brain-type) or the octamer (for Mitochondrial-type). Subjectively, which protein has a more highly conserved subunit interface? Any answer is fine!

beta sheet

It is a bit hard to tell, but there is a larger subunit interface for Mitochondrial-type CK, and the surface seems to be characterized by more blue residues. Thus, the subunit interface of the large octamer might be more conserved than the dimer interface.

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