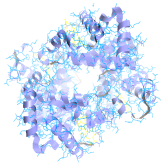

StarBiochem User Manual

Learn how use StarBiochem

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Welcome to StarBiochem

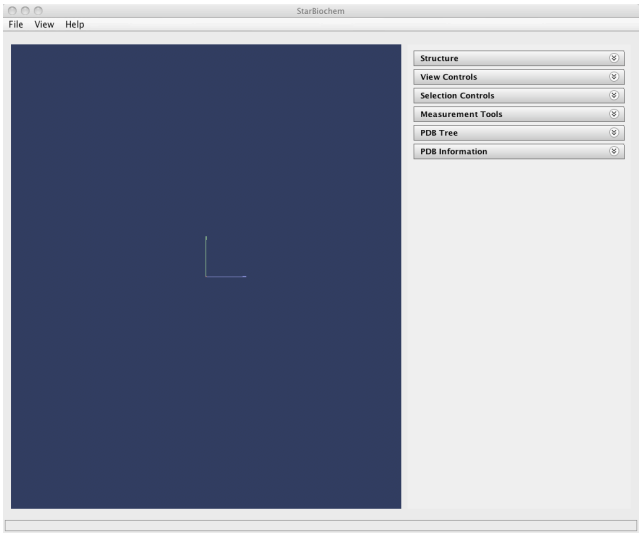
StarBiochem is a protein 3D viewer. StarBiochem runs on standard Linux, Windows and Mac computers.

Opening StarBiochem

To get started with StarBiochem:

1. Navigate to **http://web.mit.edu/star/biochem**.
2. Click on the **Start** button to launch the StarBiochem application.
3. Click **Trust** when a prompt appears asking if you trust the certificate.

This is the view you will see when you open StarBiochem.

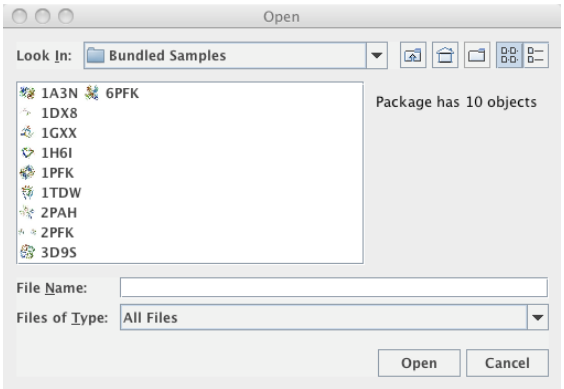


Loading a protein structure

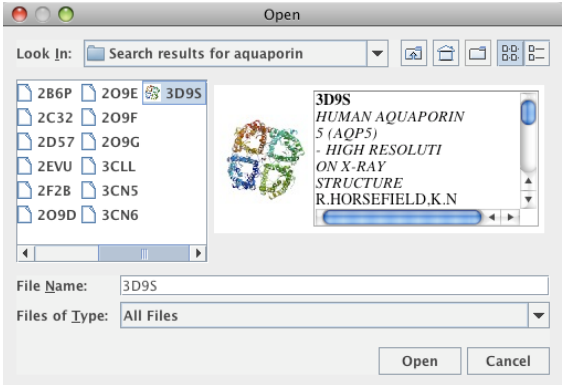
StarBiochem enables the visualization of molecules encoded within Protein Data Bank (PDB) files. PDB files are named by a four-character ID such as “1GXX”.

To open a PDB file:

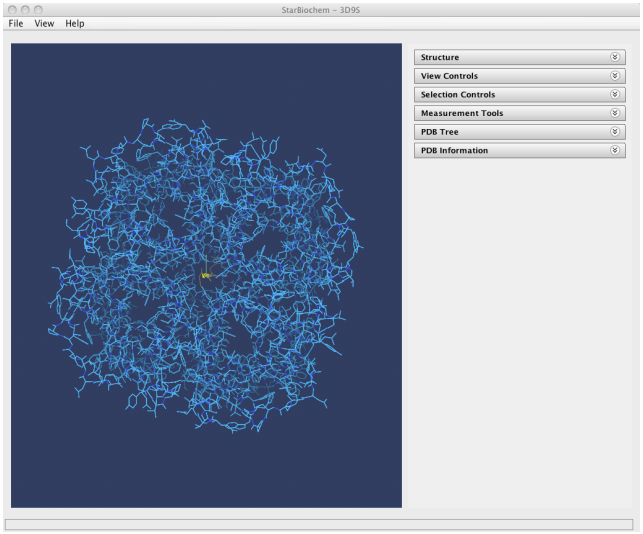
1. Click on **File -> Open/Import**.
2. In the **Look In** pull-down menu, choose a PDB file from one of the following sources:



- the **Bundled Samples** folder: click on the desired PDB file and then click **Open**.
- the **Desktop**: click on PDB file within the Desktop folder and then click **Open**.
- the PDB database via **PDB RCBS Search**: in the **Search (Keywords)** enter the PDB ID or type the name of the protein. Click on the **Search results** file within the **PDB RCBS Search** tool. Choose the desired PDB file and click **Open.**



Upon opening PDB file in StarBiochem, you will see a 3D model of the protein in the viewer.



Manipulating the default view

To rotate

Windows	**left-click** and **drag** the mouse
Mac	**click** and **drag** the mouse

To move up/down right/left

Windows	**right-click** and **drag** the mouse
Mac	**apple-click** and **drag** the mouse

To zoom

Windows	**Alt-left-click** and **drag** the mouse
Mac	**option-click** and **drag** the mouse

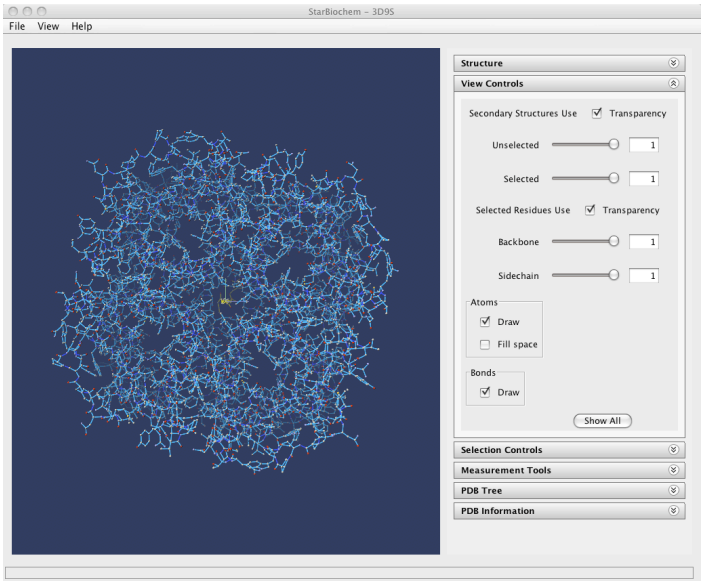
Note: sometimes you may need to zoom out to see the entire molecule after it first loads.

Visualizing atoms and bonds

The default view of a molecule is the “ball and stick” mode, where the bonds have been drawn, but not the atoms.

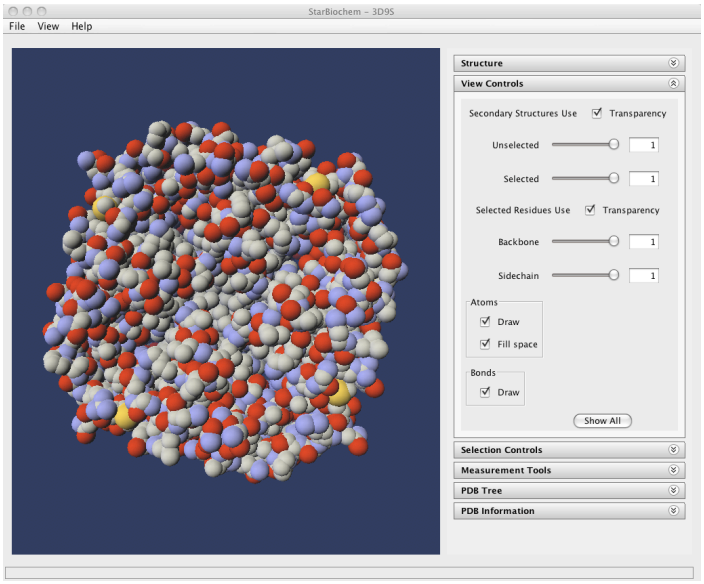
To visualize/hide atoms or bonds in the “ball and stick” view mode:

1. Click the **View Controls** panel.
2. Check the **Draw** checkbox under the **Atoms** or **Bonds** box to turn the corresponding elements or uncheck the box to turn them off.



To change the default “ball and stick” view to the “space fill” view:

1. Click the **View Controls** panel.
2. Check the **Fill space** checkbox under the **Atoms** box to display atoms in the space filled mode; uncheck the box to display them in default “ball and stick” mode.



The default coloring scheme for atoms is as follows:

- **Carbon (C) atoms** grey spheres
- **Oxygen (O) atoms** red spheres
- **Nitrogen (N) atoms** blue spheres
- **Sulfur (S) atoms** yellow spheres
- **Standard bonds** grey line segments
- **Peptide bonds** blue line segments

Note: StarBiochem does not display hydrogen atoms or water molecules contained in the PDB files.

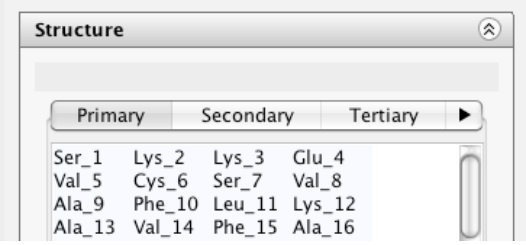
Displaying molecular structures

The **primary structure** of a protein lists the amino acids that make up a protein's sequence or the nucleotides that make up a DNA segment, but does not describe their corresponding shape. The **secondary structure** of a protein refers to how stretches of amino acids within a protein chain are arranged in space in characteristic patterns such as helices, sheets, and coils. The **tertiary structure** describes the folded shape of a protein chain and is determined by characteristic properties of the amino acid residues, such as acidic, basic, polar, and non-polar. The **quaternary structure** indicates the relationship between the chains of a molecule.

Note: for DNA segments that are crystallized with DNA binding proteins, only the primary structure of the DNA segment is shown.

Displaying primary structures:

1. Click on the **Structure**.
2. Select the **Primary** tab to display the primary structure: a numbered list of amino acids.

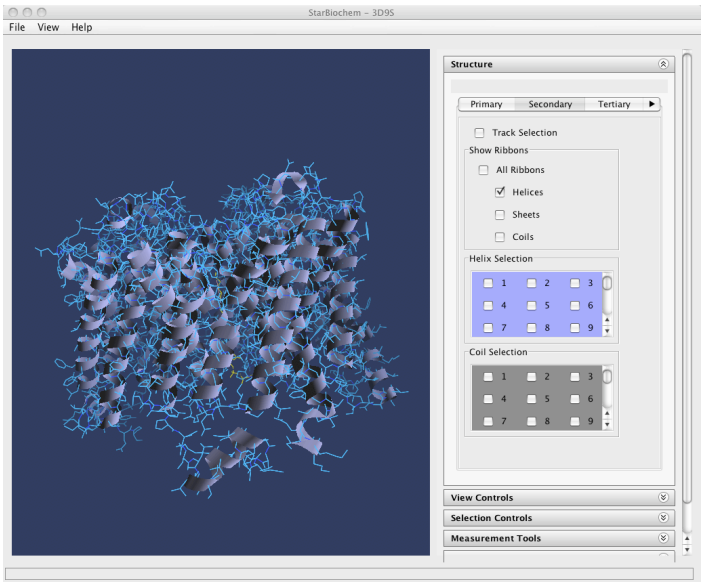


3. If necessary, scroll down through multiple numbered lists of amino acids; every list corresponds to a different protein chain (discussed later) in the molecule and is color-coded accordingly.

Left-click on a list entry to select a particular amino acid in the viewer. To select multiple amino acids, hold down **Ctrl** while clicking on them.

Displaying secondary structures

1. Click on the **Secondary** tab in the **Structure** panel.
2. Select **Helix**, **Sheet**, or **Coil**, respectively, to display secondary structures in the standard "ribbon format": ribbon-like strips in the shape of helices, sheets, or coils.



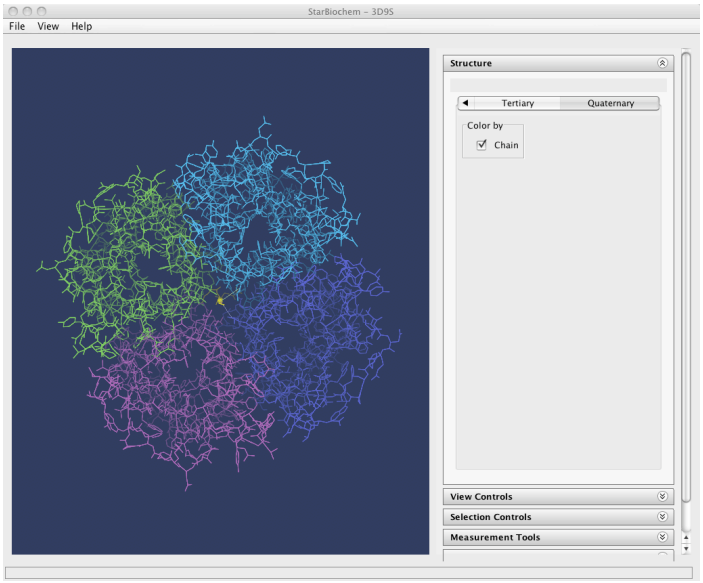
3 You can select individual helices, sheets or coils by clicking on the individual selection checkboxes for each of these secondary structures.

Displaying tertiary structures

1 Click on the **Tertiary** tab in the **Structure** panel.
2 Check a property box, e.g. **Basic**, **Acidic**, etc., to color different types of residues in the viewer.
3 Uncheck the property box to return to the default coloring scheme.

Displaying quaternary structures

1 Click on the **Quaternary** tab in the Structure panel.
2 Check the **Chain** box to color all atoms according to the chain to which they belong.



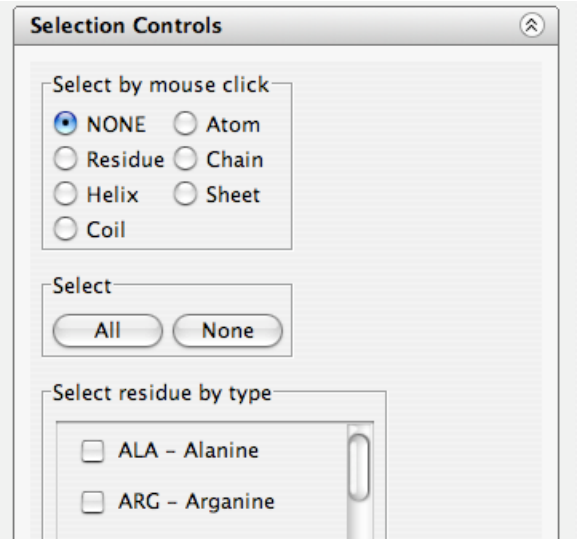
3 Uncheck the **Chain** box to return to the original color scheme.

Selecting atoms and structures

In addition to being able to select structural elements within the **Structure** controls, StarBiochem allows for selection of individual structural elements by selecting the type of element and then clicking on the actual element within the structure.

Selecting individual structural elements

1. Click on **Selection Controls** to open the panel for selecting elements of the molecule.
2. In the **Select by** groups, click on the button corresponding to the type of structural element you want to select.



3. In the viewer, click on the actual structural element to select the type of object indicated in the **Select by** boxes.
4. To select multiple atoms/sets of atoms, hold down **Ctrl** while clicking on these elements. To unselect structural elements, hold down **Ctrl** while clicking on the selected elements.

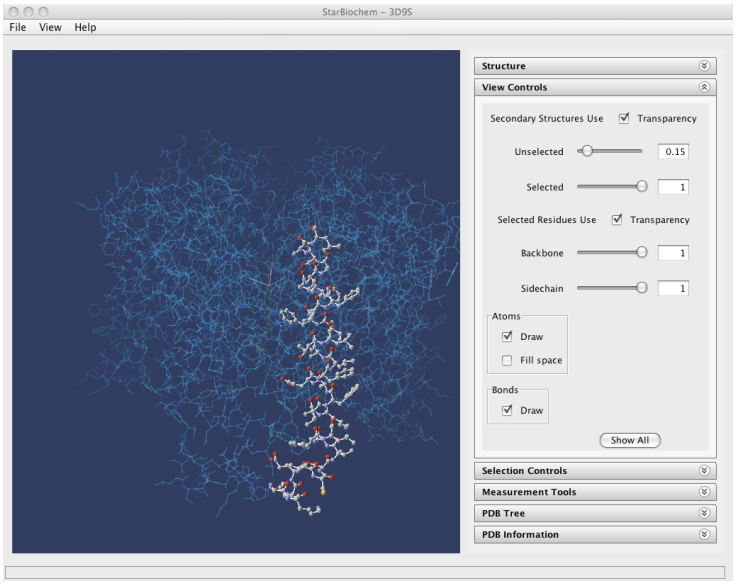
Manipulating molecule visibility

StarBiochem enables the user to focus on specific elements of the molecule by controlling the transparency of selected or unselected atoms, side chains, and backbones.

Changing visibility of selected and unselected atoms

1. Click on **Structure** to open the tabbed list of controls.
2. Navigate between the tabs to select and unselect primary, secondary, tertiary or quaternary structures.
3. Click on the **View Controls** bar to open the panel.
4. Change the visibility of corresponding atoms by manipulating the **Unselected** or **Selected** sliders or by entering a number between 0 and 1 in the boxes to the right of the sliders.

5 Check the **Secondary Structures Use Transparency** box, so that manipulating the sliders affects also the transparency of any visible secondary structures.



Changing visibility of side chains and backbones

1 Click on **Structure** to open the tabbed list of controls.

2 Navigate between the tabs to select and unselect primary, secondary, tertiary or quaternary structures.

3 In the **View Controls** panel, change the visibility of corresponding atoms by manipulating the **Sidechain** or **Backbone** sliders or by entering a number between 0 and 1 in the boxes to the right of the sliders.

4 Check the **Selected Residues Use Transparency** box, so that manipulating the sliders affects only the selected atoms.