

Opening and editing a molecular structure

Required functionality and modules: Discovery Studio Client.

Required data files: 1TPO.pdb.

Time: 10 minutes.

Introduction

Visualization and general structural analysis tools are critical in the understanding of biological and biochemical systems. Discovery Studio Client provides an interactive environment for molecular visualization, and supplies a wide range of tools for structure characterization and analysis.

A single window, the Molecule window, is provided for working with molecular structures and properties. This window has been designed to accommodate the analysis of multiple protein structures as well as large sets of small molecules. In this lesson, the emphasis is on working with protein structure data; a companion lesson focuses on dealing with molecular properties.

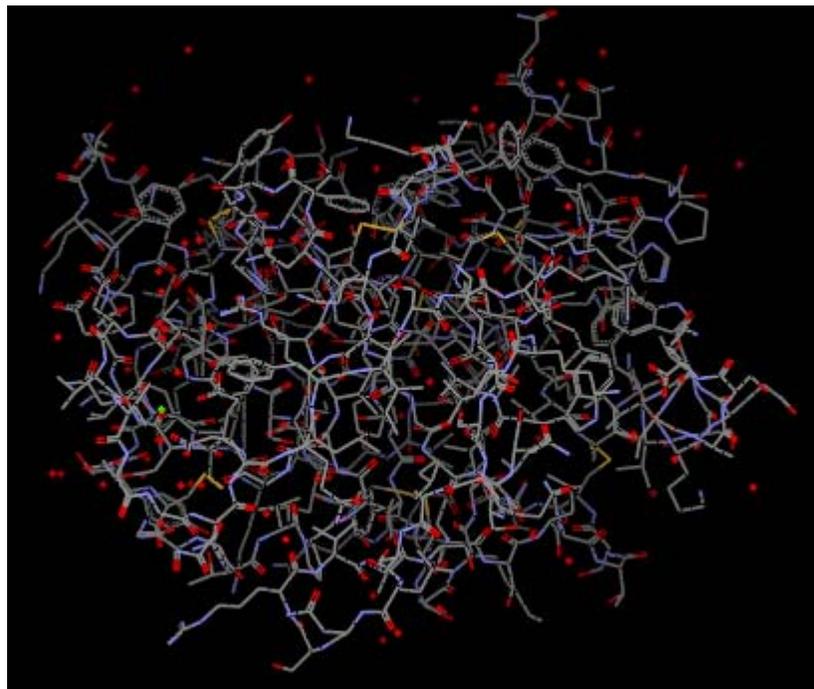
- [Opening and viewing a protein molecule in the Molecule Window](#)
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Opening and viewing a protein molecule in the Molecule Window

In this lesson, you will open a protein structure of a Serine Proteinase from a [.pdb](#) file. The PDB code for this protein is 1TPO and the sample file was downloaded from the RCSB Protein Data Bank web site.

From the Files Explorer, navigate to the **Samples** folder and open the **Tutorials | Quick Start Tutorials** subfolder. Double-click the **1TPO.pdb** file.

This opens the 1TPO.pdb file in the Molecule Window. When the 3D Window is opened a single view, the Graphics View, is displayed. The Graphics View, shows a 3D representation of the structure and is the interface used to interact with the 3D object.



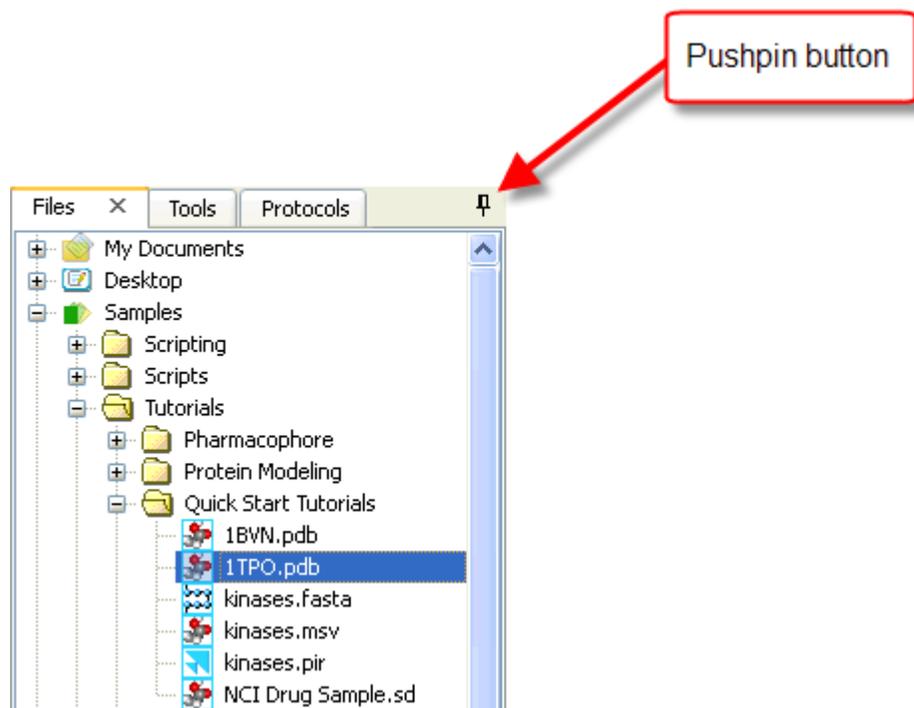
Tip. You can also quickly access the Sample folder from the Open dialog. From the menu bar, choose *File | Open...*, click the *Samples* icon on the Open dialog, choose a file from the list box, and then click *Open*.

Alternatively, if you have internet access, choose *File / Open URL...* from the menu bar to display the Open URL dialog. Enter **1TPO** (the protein PDB identifier) in the *PDB ID* text box, and then click *Open*. In this case, the 1TPO molecule is retrieved directly from the RCSB web site.

To increase the viewable area in the Molecule Window, you can use the Autohide feature of the Explorer Dock.

In the corner of the Explorer Dock, click the **Pushpin** button.

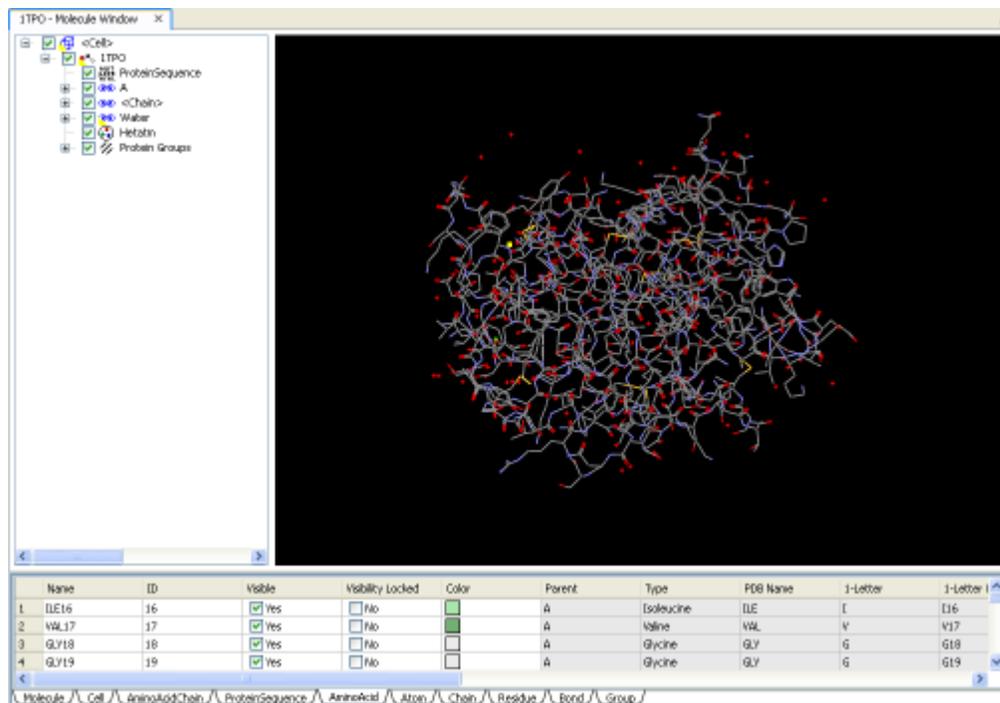
This causes the Explorer Dock to collapse and the corresponding tabs to appear on the left side of the screen. To access an Explorer Window click the corresponding tab and the Window will expand.



In addition to the Graphics View, two other views are available:

- Hierarchy View: Displays all the different objects that compose the structure (e.g., atoms, bonds, residues).
- Data Table View: Shows detailed properties of the structure in a tabular format.

To toggle the visibility of the different views, use the **CTRL+G**, **CTRL+H**, and **CTRL+T** key combinations to control the Graphics, Hierarchy and Table views respectively.



Note. Discovery Studio Client uses different settings when opening different file formats. Files not typically used to store 3D structure information, such as .sd or .smi formats, open with only the Data Table View by default. Files that are primarily used for storing structural information, such as .pdb, open with only the Graphics View by default. You can change the preferences for how certain file types are opened from the [Default Layouts](#) subpage of the Preferences dialog.

Click the **1TPO - Molecule Window** tab to make it active.

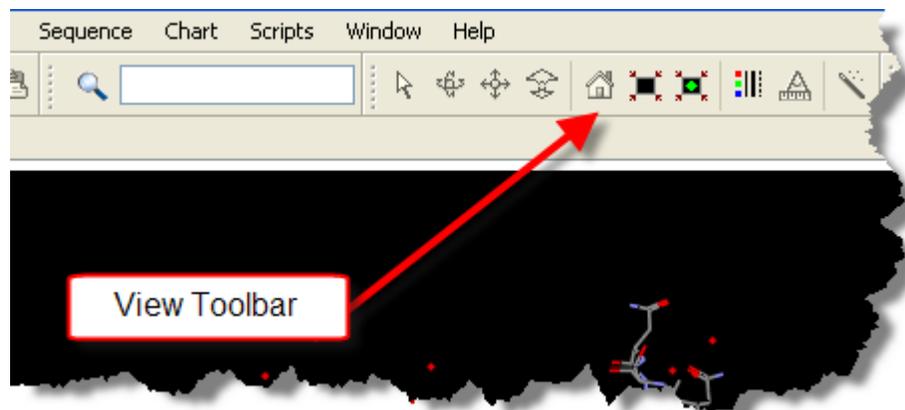
Tip. To maximize the viewing area for an active window (Molecule Window, Sequence Window, Ramachandran Plot, etc.), press F11. Press F11 again to restore your original view.

Exploring the toolbar buttons and the mouse

Click each of the following buttons on the **View** toolbar in turn and then click down the left mouse button and drag the cursor in the Graphics View.

Hover the cursor over each button on the *View* toolbar to display the tooltip that describes that button's function.

You can manipulate the view by clicking and dragging in the Graphics View of the Molecule Window.



Select: Allows you to select items in the 3D Window. Click and drag the lasso around a portion of the structure to select it. You can add to the current selection by pressing SHIFT and encircling another region with the lasso.



Rotate: Allows you to rotate the view of the structure in the Graphics View. Hold SHIFT while dragging to rotate in the Z plane. You can also rotate while in translation or zoom mode by right-clicking and dragging.



Translate: Allows you to translate the structure in the Graphics View. Click and drag to translate the molecule in the XY plane. Hold SHIFT while dragging to translate along the Z axis.



Zoom: Allows you to enlarge or reduce the view of the structure. Zoom in by dragging upward and zoom out by dragging downward.

Notes:

To adjust the position of selected atoms exclusively, hold CTRL while in rotation, translation, or selection mode.

Use CTRL+Z to revert an action such as rotation or translation.

Other mouse tools are available when you display other toolbars (e.g., the *Torsion* tool on the *Sketching* toolbar).

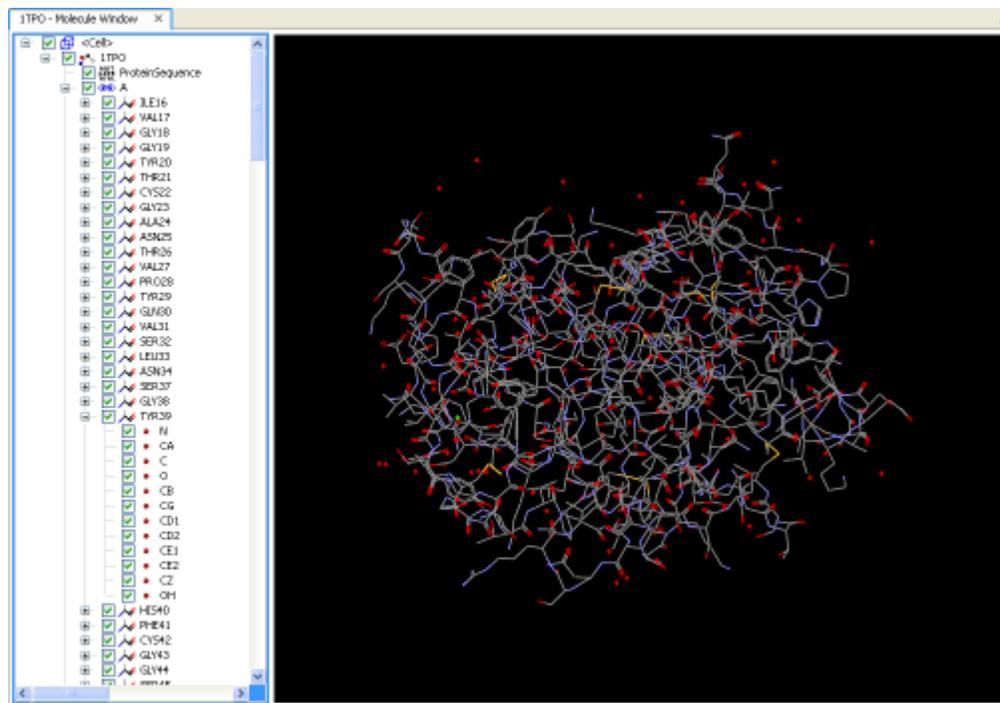
Click the **Select** tool on the **View** toolbar.

Click an **atom** in the Graphics View to select it.

Double-click the **selected atom** while it is highlighted (displayed in yellow) to select its parent residue.

Double-click the **selected residue** again while it is still selected to select its parent chain.

This allows you to progressively select different levels in the molecular hierarchy. Note that the current selection is also reflected in the Hierarchy View.



If the Hierarchy View is not visible, press **CTRL+H** to display it. Alternatively, choose **View | Hierarchy** from the menu bar.

Tip. You can cancel the selection by clicking another object to make a new selection, or by clicking an empty area in the Graphics View to select nothing.

To change the display style

Click the **1TPO - Molecule Window** tab to make it active.

Click the **Display Style** button on the **View** toolbar.

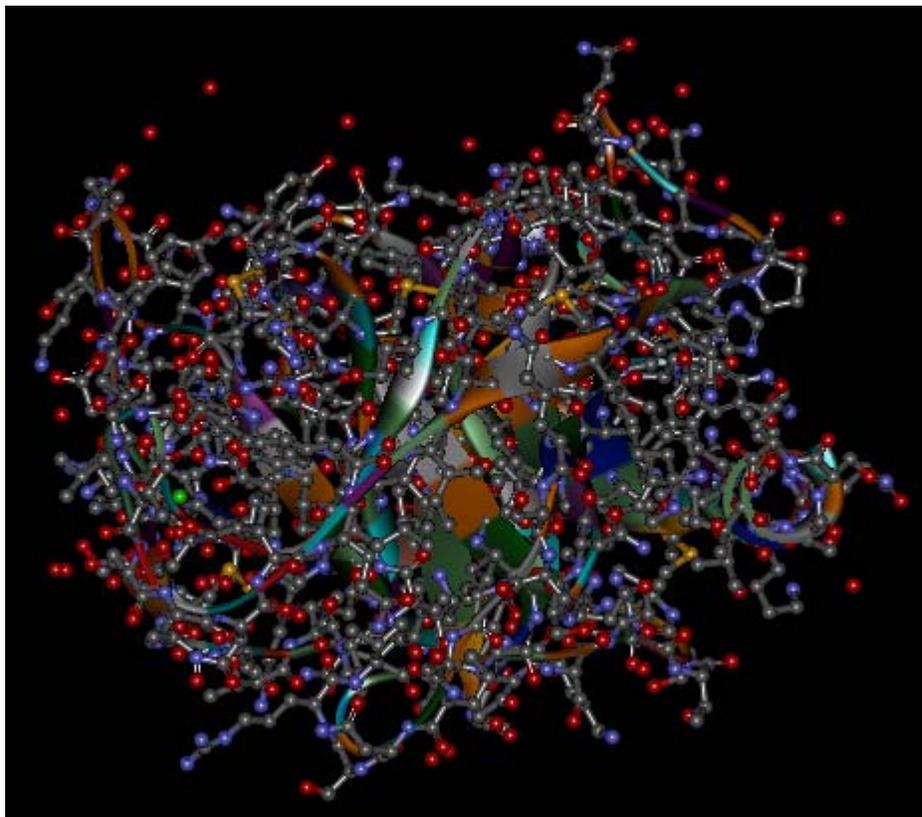
Tip. Alternatively, press CTRL+D or right-click and choose *Display Style...*

On the Display Style dialog, click the **Atom** tab.

Select the **Ball and stick** option in the **Display style** group.

Click the **Protein** tab, and then select **Solid ribbon** in the **Display style** group.

Click **OK** to apply the changes.



The atoms in the residues are displayed as solid spheres and the bonds as cylinders. The protein backbone is represented as a solid 3D ribbon.

Tip. You can use the Graphics View Display Style dialog to change the coloring of atoms and residues in the protein based on a wide range of properties.

Note. Available options on the Display Style dialog differ depending upon which window or view is current. Changes made to the display rendering only apply to selections made in the Graphics View. If nothing is selected, a general rendering change will be made.

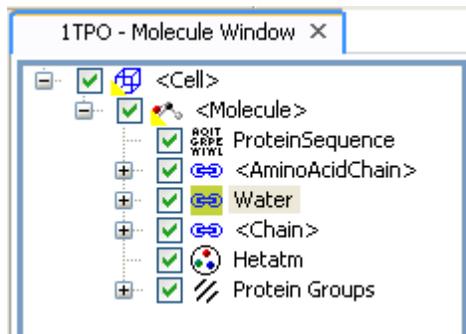
Using the Hierarchy and Data Table Views

Elements of the system can be copied, pasted, or deleted by highlighting and selecting commands from the *Edit* menu. Standard Windows shortcuts such as CTRL+C and CTRL+V can be used to quickly access this functionality.

Use **CTRL+H** to ensure the Hierarchy View is visible.

Select each of the **Water** chains from the Hierarchy View and press **DELETE** to remove these from the structure. (There are two Water chains in this structure).

Alternatively, you can select the Water chain and choose *Edit / Delete* from the menu bar.



Water molecules in the protein crystal structure are grouped into distinct chains. By deleting these chains, you can focus on the protein structure itself.

To explore views

Click the + and - symbols in the Hierarchy View to expand and contract sections of the hierarchy.

Tip. You can use the Hierarchy View to drill down to the atomic level and highlight specific atoms or groups of interest (e.g., hydrophobic residues).

Choose **View | Data Table** from the menu bar.

Tip. You can also access the Data Table View by pressing CTRL+T.

Name	ID	Visible	Visibility Locked	Color	Parent	Type	PDB Name	1-Letter	1-Letter
ILE16	16	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	■	A	Isoleucine	ILE	I	I16
VAL17	17	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	■	A	Valine	VAL	V	V17
GLY18	18	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	■	A	Glycine	GLY	G	G18
GLY19	19	<input checked="" type="checkbox"/> Yes	<input type="checkbox"/> No	■	A	Glycine	GLY	G	G19

Explore the tabs in the Data Table View and notice the association between the organization of the Hierarchy and Data Table Views (e.g., the cell and molecule levels).

Click the **Molecule** tab in the Data Table View.

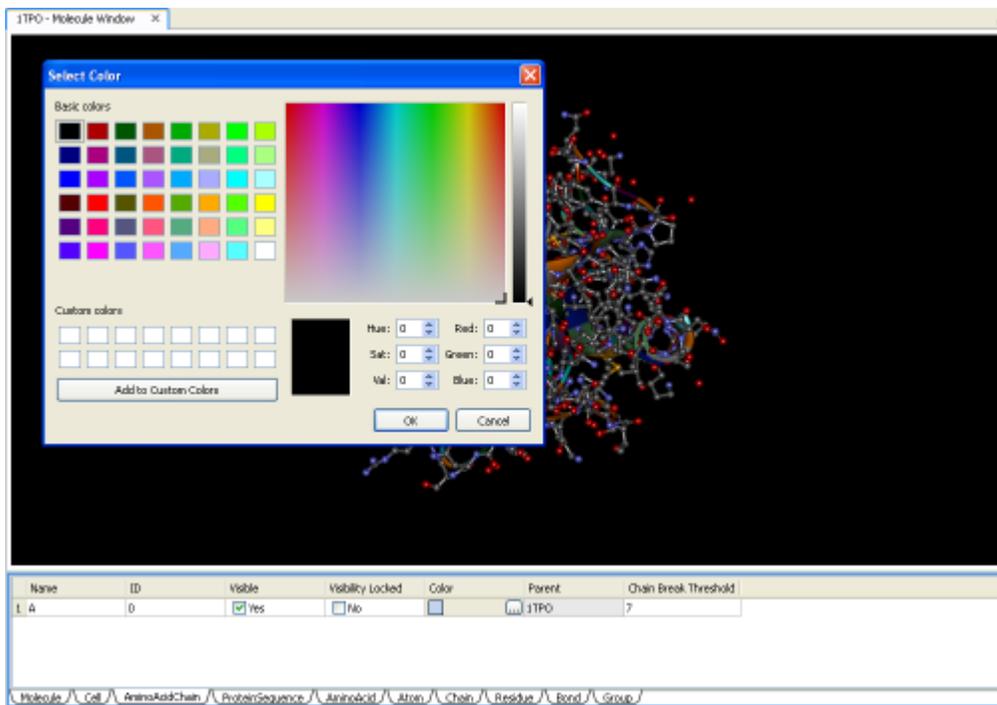
Click the header of the **Molecular Weight** column (located in the middle of the tab), and then drag and drop the header onto the **Number of Atoms** column (located at the beginning of the tab).

The order of the columns on the *Molecule* tab changes, with the *Molecular Weight* column now positioned before the *Number of Atoms* column.

Click the **AminoAcidChain** tab.

Click in the cell in the **Color** column, and then click the ... button.

This displays the Select Color dialog.



Select a **new color**, and then click **OK**.

This changes the color of the amino acid chain.

Note. The white cells in the Data Table View contain properties that can be modified, whereas the values in the gray cells cannot be edited.

Saving Files

Once you have completed modifications to the appearance of the system, you can save the modified display information by in the Discovery Studio Client file format, .dsv. Saving data in this format ensures that all changes made in the application are preserved and the data reopens in an identical state.

Choose **File | Save As...** from the menu bar.

Set the location and name of the output file.

Set the **Files of type** to **Discovery Studio Files (*.dsv)**

Click **Save**.

Note. If the data is to be used in another application that cannot read .dsv files, be sure to save a copy in a supported format.