

Common Operations in Maestro 9.3

Viewing Structures

Rotate xy: Middle button

Rotate z: Ctrl+middle button

Fix rotation in x or y direction: Shift+middle button and move mouse up or down for x and left or right for y.

Translate xy: Right button


Translate z: Ctrl+right button

Fix translation in x or y direction: Shift+right button and move mouse up or down for x and left or right for y.

Zoom: Middle+right button or mouse scroll wheel.

Spot Center: Right-click an atom to center the view and rotation around it.

Stereo view: Ctrl+S to turn stereo view on and off.

Save and restore views: Click the  button in the **Saved Views Toolbar**, or choose **View > Save View**. To restore a view, click the numbered icons in the **View Toolbar** (1, 2, 3, etc) or choose **View > Manage Views**.



Working with Projects

Create a new project: Ctrl+N

Open an existing project: Ctrl+O or click the  button in the **Project Toolbar**.

Close a project: Ctrl+W

Save a project: Choose **Project > Save As**. Subsequent work is saved automatically.

Undo/Redo: Ctrl+Z or use the  /  buttons in the **Edit Toolbar**.

Display shortcut menus: Right-click and hold in an empty portion of the **Workspace**, on an **Atom** or **Bond**, in the **Sequence Viewer**, or on **Project Table** rows or column headers.

Using the Project Table

Open the Project Table: Ctrl+T or click the  button in the **Project Toolbar**.

Include and exclude structures: To include only a single entry (row) from the **Project Table** in the **Workspace**, click the box next to that entry's name in the **Project Table**. Shift-click to include a range of entries in the **Workspace**; Ctrl-click to add or remove an entry.

Scroll up/down: Up/down arrow keys


Scroll up/down one page: Page Up / Page Down

Jump to top/bottom of the Project Table: Home/End

Jump to previous/next included entry: Ctrl+Page Up/Down

Jump to previous/next selected entry: Shift+Page Up/Down

Include the next or previous selected entry in the Workspace: Right arrow or left arrow, respectively.


Display entry information in the Workspace: Click the  button in the **Labels Toolbar** or press the S key to display single-entry feedback. To change which properties are displayed, right-click on a column header and choose a **Workspace Feedback** option from the menu that appears.


Fix selected entry in the Workspace: Right-click an entry and select **Fix**.



Include only selected entries in Workspace: Ctrl+N while the mouse pointer is over the **Project Table**.


Exclude selected entries from Workspace: Ctrl+X while the mouse pointer is over the **Project Table**. This will not delete any entries from the **Project Table**.

Working with Multiple Structures

Import single or multiple structures: Ctrl+I or click the  button in the **Project Toolbar**.



Clear the workspace: Click the  button in the **Workspace Toolbar**. This does not delete any rows (entries) in the **Project Table**; it only excludes them from the **Workspace**.

Move one molecule while keeping others fixed: Press Ctrl+G or click the  button in the **Edit Toolbar** then select molecules for local transformation. Press Ctrl+G or click the  button again to leave local transformation mode. After selecting atoms for local transformation, holding down the space bar will toggle between global and local mode.


Tile entries: Ctrl+L or click the  button in the **View Toolbar**.


Finding and Selecting Structures

Find structures or entries: Ctrl+F will display the **Find toolbar** in either the **Workspace** or **Project Table**. Use Alt+N and Alt+P to traverse matches.

Select atoms in the Workspace: Click the  button in the **Edit Toolbar** or press the ` key to enter selection mode. Drag the mouse pointer over atoms in the **Workspace** to select them. Click and hold the  button to choose whether **Workspace** selections capture atoms, residues, molecules, chains, or entries.


Working With Surfaces and Hypotheses in the Project Table

Open the Manage Surfaces panel for a given entry: Click  in the right-hand side of the **Title** column.


Open the Manage Hypothesis panel for a given entry: Click  in the right-hand side of the **Title** column.


Building and Modifying Structures


3D Building: Click **Build** in the **Manager toolbar** to display the **Build Toolbar**.


2D Building: In the **Edit toolbar**, click the  button to open the **2D sketcher**.

Add hydrogens: Double-click the **+H** button in the **Edit Toolbar** to add missing hydrogens to all structures in the **Workspace**.


Adjust torsions: Click the  button in the **Edit Toolbar**, and then click on a bond to select it. Click and drag left or right to adjust the torsion.


Create entry from Workspace: Click the  button in the **Workspace Toolbar**.


Measurements: Press and hold the  button in the **Labels Toolbar**.


Structure sculpting: Click the  button in the **Build toolbar**, then click and drag on an atom in the **Workspace**.

Using the Style Toolbar

Workspace Style: Click and hold the  button to define visual styles. Click the button once to apply the currently defined style to the entire **Workspace**.

Automatically apply style: Click the  button to automatically reapply the workspace style whenever the contents of the workspace change.

View interactions: Click the  button to display H-bonds and contacts.

Create surfaces: Click the  button to create ligand or binding-site surfaces. Click and hold the button to show or hide existing surfaces.

Keyboard and Toolbar Shortcuts in Maestro 9.3

Project Operations

Show/Hide Project Table: **Ctrl+T**

New project: **Ctrl+N**

Open project: **Ctrl+O**

Close project: **Ctrl+W**

Import structures: **Ctrl+I**

Cut: **Ctrl+X**

Copy: **Ctrl+C**

Paste: **Ctrl+V**

Paste by placing: **Ctrl+Shift+V**

Undo: **Ctrl+Z**

Open Command Script Editor: **Ctrl+E**

Create Project Table entry from contents of Workspace: **Ctrl+Shift+N**

Mark target entry: **X**

Display single-entry feedback in Workspace: **S**

Quit Maestro: **Ctrl+Q**

Open help page for active panel: **F1**

Open online help: **Ctrl+H**

Modifying Structures

Toggle between local and global transformation: **Ctrl+G**

Delete selected atoms: **Del**

Clean up geometry: Press **U** to perform a quick minimization with loose convergence criteria.

Minimize structures in the Workspace: Press **Ctrl+M** to perform a more thorough minimization.

Using Atom Sets

Save selected atoms as Atom Set 1: Press **Ctrl+1**. **Ctrl+0** through **Ctrl+9** work similarly.

Select atoms from Atom Set 1: Press **1**. Keys **0** through **9** work similarly.

Workspace Operations

Full screen Workspace mode: Press **Ctrl+=**. Press **Esc** or **Ctrl+=** to exit.

Apply Workspace style: **Ctrl+Y**

Tile Workspace: **Ctrl+L**

Transform all tiles: **Ctrl+Shift+L**

Fit to selected atoms: Press **Z**. If no atoms are selected, all Workspace contents will be fit to screen.

Fit ligand to Workspace: **L**

Zoom in: **K**

Zoom out: **J**

Move clipping planes back: **-**

Move clipping planes forward: **+**

Move clipping planes together: **F**

Move clipping planes apart: **G**

Toggle enhanced depth view on/off: **D**

Stereo view: **Ctrl+S**

Go to previous/next scene: **Ctrl+Shift+.** and **Ctrl+Shift+,**

Finding and Selecting Atoms

Find substructures or entries: **Ctrl+F**. **Alt+N** and **Alt+P** select next and previous matches.

Activate atom selection tool: **`**

Select clicked atoms: **A**

Select clicked bonds, residues, chains, molecules, or entries: **B**, **R**, **C**, **M**, or **E**, respectively.

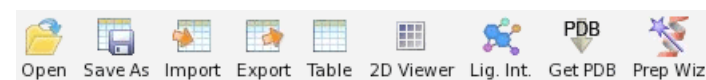
Select all: **Ctrl+A**

Saving Views and Scenes

The Saved Views toolbar can be used to save and restore specific vantage points in the Workspace. To save and restore the contents of the Workspace, use the **Workspace > Scenes > New** and **Workspace > Scenes > Manage** menu items.

Toolbar Guide

Project



Edit



View



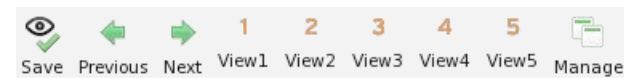
Workspace



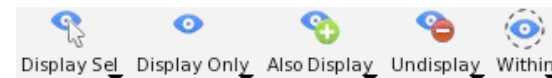
Style



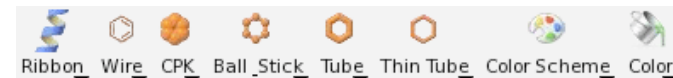
Saved Views



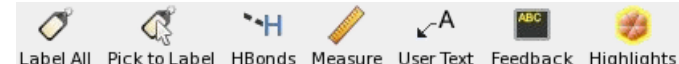
Display Atoms



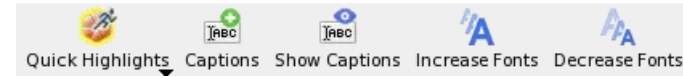
Representation



Labels



Build



Fragments

