

# Maestro 9.9

## User Manual

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# Document Conventions

In addition to the use of italics for names of documents, the font conventions that are used in this document are summarized in the table below.

Font	Example	Use
Sans serif	Project Table	Names of GUI features, such as panels, menus, menu items, buttons, and labels
Monospace	<code>\$SCHRODINGER/maestro</code>	File names, directory names, commands, environment variables, command input and output
Italic	<i>filename</i>	Text that the user must replace with a value
Sans serif uppercase	CTRL+H	Keyboard keys

Links to other locations in the current document or to other PDF documents are colored like this: [Document Conventions](#).

In descriptions of command syntax, the following UNIX conventions are used: braces { } enclose a choice of required items, square brackets [ ] enclose optional items, and the bar symbol | separates items in a list from which one item must be chosen. Lines of command syntax that wrap should be interpreted as a single command.

File name, path, and environment variable syntax is generally given with the UNIX conventions. To obtain the Windows conventions, replace the forward slash / with the backslash \ in path or directory names, and replace the \$ at the beginning of an environment variable with a % at each end. For example, `$SCHRODINGER/maestro` becomes `%SCHRODINGER%\maestro`.

Keyboard references are given in the Windows convention by default, with Mac equivalents in parentheses, for example CTRL+H (⌘H). Where Mac equivalents are not given, COMMAND should be read in place of CTRL. The convention CTRL-H is not used.

In this document, to *type* text means to type the required text in the specified location, and to *enter* text means to type the required text, then press the ENTER key.

References to literature sources are given in square brackets, like this: [10].



---

# Maestro Overview

Maestro is the graphical user interface (GUI) for nearly all of Schrödinger's computational programs: BioLuminate, CombiGlide, ConfGen, Core Hopping, Desmond, Epik, Field-based QSAR, Glide, Impact, Jaguar, Liaison, LigPrep, MacroModel, MCPRO<sup>+</sup>, Phase, Prime, PrimeX, QikProp, QSite, SiteMap, Strike, and WaterMap. It contains tools for building, displaying, and manipulating chemical structures; for organizing, loading and storing these structures and associated data; and for setting up, submitting, monitoring, and visualizing the results of calculations on these structures. Maestro's Job Control facility manages jobs submitted from Maestro and from the command line to both local and remote hosts. Maestro can be run locally and submit jobs to any host that you have access to.

The Maestro interface uses the OpenGL graphics tools, and can take advantage of hardware graphics capabilities, including stereo viewing capabilities. Maestro runs on Linux, Mac and Windows platforms. For information on Maestro requirements, software and hardware, see [Chapter 2](#) of the *Installation Guide*. For information on configuring stereo viewing, see [Section 4.7](#) on page 74.

This manual contains an introduction to the Maestro graphical user interface (GUI) and a description of how to use Maestro's settings, panels, and features to build, import, and manipulate molecular structures. No prior knowledge of Maestro is assumed. If you cannot find the information you are looking for in this document, see the Maestro online help. For help with preparing and starting computations, see the user manual for the related product. For help with Job Control, see the *Job Control Guide*.

This chapter provides an overview of Maestro—the general interface design, Maestro projects, Maestro workflow, and running jobs from Maestro.

## 1.1 General Interface Design

The Maestro interface is built on the Qt toolkit, and inherits many standard features from Qt. The design follows most common interface conventions, but it has some characteristics that are unique. The general operation of the Maestro interface is described in this section. Specific features are described in the relevant sections or chapters.

### 1.1.1 Maestro Windows

Maestro is based on a main window, from which you can open a range of secondary windows for the performance of various tasks. The main window is described in detail in [Chapter 2](#).

Most of the windows that are opened from Maestro are amodal, and are called *panels*. More than one panel can be open at any given time, and a panel need not be closed for an action to be carried out. Some of the panels are docked by default into the main window. You can undock them and place them wherever you want, and you can redock them, using the docking button.



If you do not want the panels to be docked, deselect Allow docking of panels under General → Panels in the Preferences panel (see [Section 14.1.6 on page 335](#)). Panels can be closed with CTRL+W or the close button on the title bar.

Maestro also has dialog boxes, most of which are modal: you must click OK to carry out the action and you cannot open any of the panels while the dialog box is open. There are also some dialog boxes that allow you to carry out limited operations in the Workspace or in a panel.

### 1.1.2 Mouse Functions

Maestro supports common mouse functions:

- The left button (button 1) is used for selecting: choosing menu items, clicking buttons and selecting objects. This button is also used for resizing and moving panels. In the description of mouse actions, “click” always means left-click.
- The right button (button 3) is used for opening a shortcut (context-sensitive) menu, where these menus are available.
- Shift-click is used to select a contiguous range of items in a list, and control-click is used to select and deselect a single item in a list without affecting the selection of other items.
- Dragging operations are supported. For instance, in the Workspace, dragging selects multiple objects. In the Project Table, dragging selected entries allows you to reposition the entries; dragging a column heading moves the column; dragging on the boundary of a row or column resizes the row or column.
- The scroll wheel is supported for scrolling vertically in tables, lists, and text areas. In lists, scrolling is equivalent to using the UP ARROW and DOWN ARROW keys. In tables, the table scrolls one line at a time, or, with the SHIFT key, one page at a time.

There are also specialized mouse functions in the Workspace, which are described in [Section 2.8 on page 32](#).

If the handedness on your mouse is set to “left”, the mouse functions are the opposite of those described: the right button is used for picking, and the left button is used for shortcut menus.

Maestro is designed for the use of a three-button mouse, but provides settings for a two-button mouse and a trackpad, which are automatically detected and applied.

You can customize the mouse button actions in the Customize Mouse Actions panel—see [Section 13.3 on page 317](#) for details.

### 1.1.3 Keyboard Shortcuts and Shortcut Menus

Maestro supports keyboard shortcuts in some of its panels, including the main window. These shortcuts are documented with the relevant panel. The shortcut keys do not work if you have NUM LOCK, CAPS LOCK, or SCROLL LOCK enabled.

The PAGE UP, PAGE DOWN, HOME, and END keys are supported in tables.

The F1 key opens the help topic for the panel, and is equivalent to clicking the Help button.

Panels that are not docked into the Workspace can be closed with CTRL+W.

Maestro supports the use of shortcut menus, which are opened by right-clicking. A standard set of menu items, along with the corresponding keyboard shortcuts, is available in any text input area: Undo (CTRL+Z, ⌘Z), Redo (CTRL+SHIFT+Z, ⇧⌘Z), Cut (CTRL+X, ⌘X), Copy (CTRL+C, ⌘C), Paste (CTRL+V, ⌘V), Delete, and Select All (CTRL+A, ⌘A).

### 1.1.4 File and Directory Selection

The Maestro dialog box that is used for selecting a file, a project, or a directory is a fairly standard file selector, but also has some custom features, some of which depend on the particular task to be performed with the file. File selectors contain the following features:

- Path option menu—This option menu lists all the parents in the current path, as well as recent locations (the path history). You can use this option menu to select the directory whose contents are displayed in the area below. The latest directory choice is displayed as the selected item in this menu.
- Navigation buttons—These buttons allow you to navigate through the history of the directory choices made, navigate up to the parent directory, or create a new subdirectory (folder) in the current directory.
- View buttons—These buttons allow you to switch between a list view and a view that provides details on the files and directories listed.

- Standard directories—This area contains labeled icons for the standard locations for a file. When you select one of these items, the path option menu is updated and the list of files and folders is updated.



Set the path to your home directory. This is `$HOME` on Linux (usually `/home/username`) and Mac (`/Users/username`), and `%HOME%` on Windows (usually the same as `%USERPROFILE%`).



Set the path to the a custom directory, which is created if it does not exist. See [Section 14.1.2 on page 332](#) for information on customizing this location. The default is the Maestro [startup directory](#).



Set the path to the Maestro current working directory. This is the [startup directory](#) unless you have set a preference for another directory, or changed the current working directory.

*Windows only:*



Set the path to My Computer.



Set the path to My Documents.



Set the path to the Desktop.



Set the path to My Network Places.

- List of current directory contents—This area lists the files and directories (folders) in the current choice of directory. To select multiple items, use shift-click and control-click. To scroll to files or folders that begin with a particular character, press the key for that character. The first file or folder beginning with that character is selected (and anything else is deselected). To sort the files, click in the heading of the column you want to sort by.
- File name text box—Displays the name of the file or files. Multiple items are listed in quotes, separated by a space. You can type the file names in to this text box, with either an absolute or a relative path, and press `ENTER` to perform the action. You can also type in a path and press `ENTER` to change directories.

This text box supports inline completion, and by default contains the last item selected. To replace the text that is already there, simply type over it. When what you type does not match anything in the current directory, the completion text disappears.

- Files of type option menu—Lists the valid file names with their extensions. Choosing an item on this option menu limits the display of the directory contents to files of the specified type.



If you choose Custom File Filter, a dialog box opens in which you can specify a filter for the files that are displayed. The filter supports the common filename metacharacters and expressions:

- \* Match any string of zero or more characters
- ? Match any single character
- [*chars*] Match any one of the enclosed characters
- {*string1,string2,...*} Match one of the enclosed strings in the comma-separated list

- Action buttons—Along with the standard Cancel and Help buttons, there is an action button for the action to be performed on the file. The most common action buttons are Save and Open.

Directory selectors are similar, except that the File name text box is now a Directory text box, and the Files of type option menu choice is Directories, and cannot be changed.

Project selectors are the same as file selectors, with the Files of type option menu choice set to select Maestro projects.

When you first open a dialog box to choose a file, project, or directory, the [current working directory](#) is the directory (folder) whose contents are displayed. If you navigate to some other location in the dialog box, the dialog box remembers this location and uses it the next time it is opened in the current Maestro session. It is not subsequently affected by changes in the current working directory.

## 1.2 Maestro Workflow

The main Maestro workflow involves performing actions on the displayed structures, to change the appearance of the structures or to change the content of the structures. In many cases, you will want to change only a part of the structure, which involves selecting the atoms that you want to change. (The workflow for a product, which is supported by Maestro panels, involves setting up and running jobs.)

Maestro has two ways of performing an action on a structure or a part of a structure:

- Choose an action first and then select the atoms to apply the action to.

Actions are usually chosen either from a toolbar button menu or by opening a panel and selecting options.

- Select atoms first and then choose an action to perform on them.

Actions can be performed by opening a panel, selecting options and clicking the Selection button, or by choosing an item from the selection shortcut menu. See [Section 2.7 on page 27](#) for more details on this shortcut menu.

Maestro's atom selection tools provide you with a range of options for selecting single atoms, entire structural units, or complex combinations of atom sets. These tools are described in detail in [Chapter 6](#).

## 1.3 Maestro Projects

When you use Maestro, you are always working in a *project*. A project is a collection of chemical structures and their associated data. The structures and data are organized into *entries*, each of which can consist of multiple molecules and their properties. The project is represented in the Project Table, which displays an ordered list of entries and associated data.

You can open the Project Table panel by choosing Project → Show Table, pressing CTRL+T, or by clicking the Table button on the Project toolbar.



If you do not specify a project when you start Maestro, Maestro creates a *scratch* project. You can work in a scratch project, but you must save it in order to use it in future sessions. Scratch projects are stored in a temporary location—see [Section 14.1.2 on page 332](#) for more information on this location.

Row	In	Stars	Title	Entry ID	Date Added	Date Modified	prepared	docking score	g
1	<input type="checkbox"/>	☆☆☆☆	1fjs_prep_lig	1	2014-01-2...	2014-01-27 1...			
2	<input type="checkbox"/>	☆☆☆☆	1fjs_prep_recep	2	2014-01-2...	2014-01-27 1...	<input checked="" type="checkbox"/>		
			1 - factorXa_sp_pv [51]						
3	<input checked="" type="checkbox"/>	☆☆☆☆	1fjs_prep_recep	3	2014-01-2...	2014-01-27 1...	<input checked="" type="checkbox"/>		
4	<input checked="" type="checkbox"/>	☆☆☆☆	15650 Known Active	4	2014-01-2...	2014-01-27 1...		-10.264	
5	<input type="checkbox"/>	☆☆☆☆	16088 Known Active	5	2014-01-2...	2014-01-27 1...		-10.096	
6	<input type="checkbox"/>	☆☆☆☆	1167 Known Active	6	2014-01-2...	2014-01-27 1...		-9.004	
7	<input type="checkbox"/>	☆☆☆☆	15722 Known Active	7	2014-01-2...	2014-01-27 1...		-8.736	
8	<input type="checkbox"/>	☆☆☆☆	700000	8	2014-01-2...	2014-01-27 1...		-8.108	

Entries: 53 total, 50 selected, 2 included Groups: 1 total, 0 selected Properties: 290 total, 259 shown

Figure 1.1. The Project Table panel.

Entries are represented by rows in the Project Table. Each row contains the row number; the entry's Workspace inclusion state (the In column); the title; a set of buttons (in the Title column) to open panels if there is auxiliary data associated with the entry such as surfaces, trajectories, vibrations, hypotheses; the entry ID, and any properties associated with the entry.

You control which entries are displayed in the Workspace from the Project Table. You can use entries as input for most of the computational programs. You can select entries as input for the ePlayer, which displays the selected structures in sequence. You can duplicate, combine, rename, split, and sort entries; create properties for entries, import structures as entries, and export entries in various formats. Although the Project Table does not have spreadsheet capabilities, you can export properties to and import properties from a spreadsheet.

When you build molecules in the Workspace, they constitute a *scratch* entry until you choose to save the structures as project entries. The scratch entry is not saved with the project unless you explicitly add it to the project. However, you can use a scratch entry as input for some jobs, and the results can be incorporated.

For products that have wizard-based interfaces (CombiGlide, Phase, and Prime), data is stored inside the project, grouped as entities called “runs”. Output from each step is incorporated into the next step and stored in the project, but not via the Project Table. The data in the runs can include structural data, but do not make use of the Project Table directly. Instead, structures can be copied to and from the Project Table at various points in the run.

More information on projects is given in [Chapter 9](#).

## 1.4 Access to Applications

Maestro provides panels for preparing and running jobs for most of Schrödinger's applications. Access to these applications are presented on the menu bar as two alternative menus, and also in a panel that provides extra features for finding and selecting applications. The menus are:

- **Tasks menu**—This menu lists the main tasks that can be performed by Schrödinger applications. If you know what kind of task you want to perform, you can use this menu. It is displayed by default on the menu bar in the main window. If the Applications menu is displayed, choose Task View from this menu to display the Tasks menu.
- **Applications menu**—This menu lists the available applications (products). If you are familiar with the products, you can use this menu to find the panel you want to use. To display this menu, choose Application View from the Tasks menu.

Both of these menus are also displayed in tree form with search capabilities, in the Task Tree and Application Tree panels. Like the menus, these panels are interchangeable and can be switched from the panel itself. The Task Tree panel opens by default when Maestro is started,

but you can open it by choosing Show Tree from either of the menus. A brief description of how to use the panel is given in the lower section of the panel when it first opens.

- To expand or collapse a submenu (node) in the tree, click on the + or – button.

You can also expand and collapse the submenu by right-clicking on the name and choosing Selected from the Expand or Collapse submenu, or expand a submenu and collapse all others by choosing Expand → Only Selected.

- To expand or collapse all submenus, right-click on any submenu and choose All from the Expand or Collapse submenu, or click the Settings button and choose Expand All or Collapse All.



- To display a description of a task or panel (leaf) in the lower section of the panel, click on the task or panel.

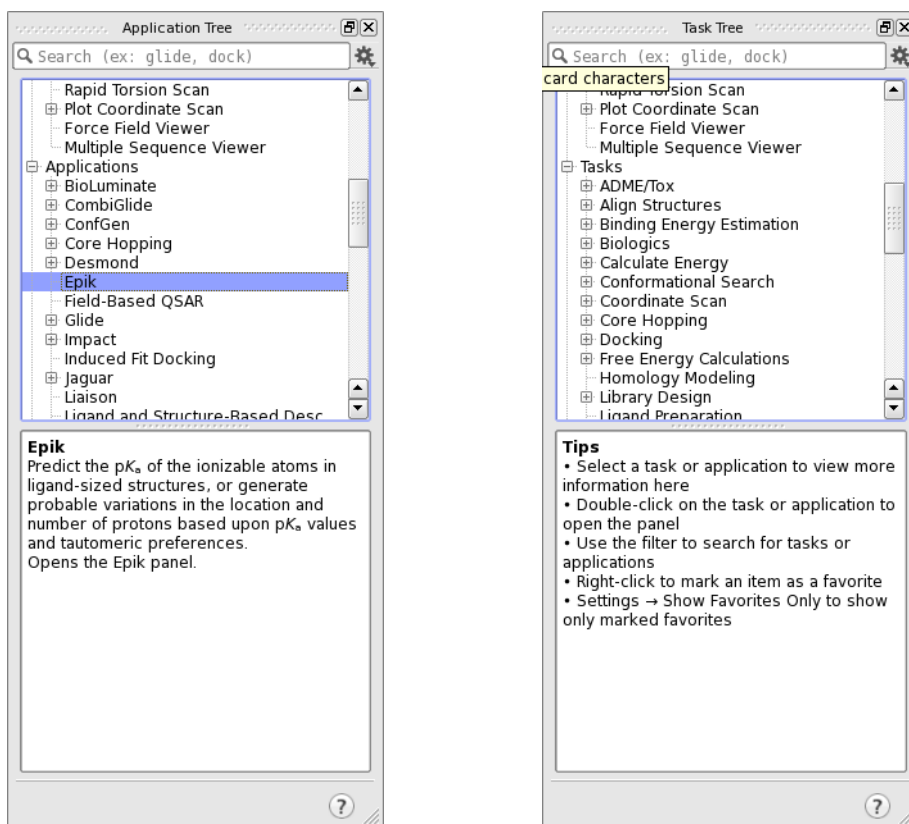


Figure 1.2. The Application Tree and Task Tree panels.

- To find a task or panel by searching the text of the menu, the name of the task or panel, or its description, enter text in the search box at the top of the panel. Only the items that contain matching text are shown in the tree. The tree is updated as you type. Click the clear (X) button in the search box to clear the search text and redisplay the full tree.
- To open a panel, double click the task or panel name, or right-click on it and choose Open.

In addition to the Tasks and Applications menus, the panel shows the Tools menu and the Scripts menu. This allows you to search more widely for the task that you are interested in.

Maestro has a large number of application panels. If your workflow only uses a few of them, or only uses a few of them most of the time, you can designate “favorite” applications, and display a tree that only contains the favorites. To mark an item as a favorite, right-click on it and select Favorite. To show only the favorites in the tree, select Show Favorites Only on the Settings button menu. The panel title is updated to reflect this choice. You can also restrict the Tasks and Applications menus to only the designated favorites by selecting Show Favorites Only on the menu. To show the full tree or menu, deselect this item.

The menus can also be customized—see [Section 13.2 on page 314](#).

## 1.5 Running Jobs

When you have set the appropriate options in an applications panel, you use the Job toolbar to start the job. This toolbar is described in all the application manuals. Briefly, you can click Run to run a job with the current job settings, or click the Settings button to open the Job Settings dialog box and set options for running the job. See [Section 2.2](#) of the *Job Control Guide* for a detailed description of the options in the Job Settings dialog box. When you have finished, click Run to launch the job (and optionally open the Monitor panel), or click save to save the settings for the next job. Note that most jobs that are run locally are automatically run at low priority so that they do not significantly affect the performance of Maestro. Exceptions are noted in this manual.

Maestro’s job launching and incorporation capabilities are designed to make it easy to manage multiple structures and their passage through multiple computational programs, without having to deal with the details of the file system. The running of jobs is handled by the Job Control facility, which is described in detail in the *Job Control Guide*.

Input files for the job are written to the *launch* directory, which is Maestro’s [current working directory](#). This directory can be changed by choosing Project → Change Directory and navigating to the new directory in the Change Directory dialog box, or by entering the command `cd path` in the Commands text box (command input area) in the main window. You can also set preferences for this directory—see [Section 14.1.2 on page 332](#).

Once a job is launched, the Monitor panel can be used to display job progress, which can also be summarized on the status bar. You can open the Monitor panel from the Tasks menu or the Applications menu, or have it open automatically on starting a job by setting a preference in the Preferences panel. You may cease or resume monitoring at any time, and you can monitor any currently running job. If a job finishes while it is being monitored, its output is incorporated into the current project, according to the settings used to launch the job. If a job that is not currently being monitored finishes successfully, you must select it in the Monitor panel and click Monitor to incorporate the results. Multiple structures are incorporated as entry groups.

Two other tools offer quick access to information on running jobs: the status button on the Job toolbar in the application panel, which you click to show a small job status window, and the Jobs button on the status bar in the main window.

For the programs that do not incorporate results, the output files are placed in the launch directory.

For information on Job Control and incorporation, see the *Job Control Guide*.

## 1.6 Citing Maestro in Publications

The use of this product should be acknowledged in publications as:

Maestro, version 9.9, Schrödinger, LLC, New York, NY, 2014.

---

# The Maestro Main Window

This chapter describes how to start and end a Maestro session, and gives a detailed description of the main window and its functions.

## 2.1 Starting Maestro

The mechanism for starting Maestro is different for Linux, Windows, and Mac hosts. This mechanism is described for each of these host types in the following subsections.

When Maestro starts, it reads resource files that define your preferences from your [user profiles directory](#). For information on the location of this directory and on setting preferences, see [Chapter 13](#). Any resource files that it does not find in this location it reads from the resource subdirectory in the Schrödinger software installation, `maestro-vversion/data/res`, where *version* is the 5-digit Maestro version number. The resource files and preferences are saved in your user profiles directory when you quit Maestro.

If you are starting a new release of Maestro for the first time, the preferences and resource files are copied from the location for the previous release. Your preferences are therefore preserved for the new version of Maestro. However, layout settings are not copied, because changes to the panels might make some controls hidden with the saved layout. If you see warnings on startup, it is likely that a customization is no longer valid, due to definitions changing between releases. For more information on defining resources, see [Section 13.5 on page 320](#).

Maestro has the concept of a *startup directory*, which on Linux is the directory from which Maestro was started. On Windows and Mac, the startup directory is set to the Schrödinger folder in your documents folder. The startup directory is used for Maestro's *current working directory*, subject to a preference (see [Section 14.1.2 on page 332](#)). To change the current working directory, you can choose Project → Change Directory and navigate to the new directory in the Change Directory dialog box.

If Maestro fails to start, the Diagnostics panel opens, with instructions about what to do about the failure. More information on this panel is given in [Section 7.6.1](#) of the *Installation Guide*.

### 2.1.1 Starting Maestro on a Windows Host

To start Maestro, double-click the Maestro icon on the desktop, or use the Start menu. Maestro is in the Schrödinger submenu. This submenu can also be used to open the release notes and the documentation index in your browser.

To start Maestro with a specific project, double-click the zipped project. Zipped projects have a `.prjzip` extension, and are read-only. To replace the zipped project, you must first save it, then zip it, then copy it over the old project. Zipped projects can also be linked to a web page: clicking on the link to the project in your browser opens the project in Maestro.

You can import a Maestro, PDB, SD or MOL2 file into a Maestro session by double-clicking on the file icon. For Maestro files, if there is an existing Maestro session open, the file is imported into this session (or the most recently used session if there is more than one).

### 2.1.2 Starting Maestro on a Mac Host

To start Maestro, click the Maestro icon on the dock. If there is no Maestro icon on the dock, you can put one there from Finder by choosing `Go → Applications` and opening the `SchrodingerSuite2014-3` folder. Icons for all the Maestro profiles (and other graphical applications) are available there, and you can drag them to the dock.

You can also start Maestro from the command line, by opening a terminal window and using the instructions given below for Linux and the bash shell.

### 2.1.3 Starting Maestro on a Linux Host

Before starting Maestro, you must set the `SCHRODINGER` environment variable to point to the installation directory, by entering the following command in a terminal window:

```
csh/tcsh:      setenv SCHRODINGER installation-directory
bash/ksh:     export SCHRODINGER=installation-directory
```

You might also need to set the `DISPLAY` environment variable, if it is not set automatically when you log in. To determine if you need to set this variable, enter the command:

```
echo $DISPLAY
```

If the response is a blank line, set the variable by entering the following command:

```
csh/tcsh:      setenv DISPLAY display-machine-name:0.0
bash/ksh:     export DISPLAY=display-machine-name:0.0
```

For local display, you should omit `display-machine-name`.

After you set the environment variables, you can start Maestro using the command:

```
$SCHRODINGER/maestro [options] [filename]
```



The options for the `maestro` command are listed in Table 2.1. You can use command options to specify a file of a particular type. The optional *filename* specifies a file to be imported into the project, in any format that Maestro recognizes by its extension.

Table 2.1. Options for the `maestro` command.

Option	Description
<code>-b PDB-file</code>	Read a PDB file. Cannot be used with <code>-m</code> .
<code>-c command-script</code>	Run the specified Maestro command script when Maestro starts, after the main window is drawn.
<code>-h</code>	Print a usage message, but do not start Maestro.
<code>-I</code>	Display extra information about X visual settings when Maestro starts.
<code>-l layout-file</code>	Use the specified layout file to define panel positions and sizes.
<code>-lsgfx</code>	List information on the graphics, if available. Linux only.
<code>-m filename</code>	Load structures from a Maestro ( <code>.mae</code> ), compressed Maestro ( <code>.mae.gz</code> or <code>.maegz</code> ) or MacroModel ( <code>.dat</code> ) structure file. Cannot be used with <code>-b</code> .
<code>-nosplash</code>	Disable display of the splash screen when starting Maestro.
<code>-p project</code>	Load the specified Maestro project. Project names normally end in <code>.prj</code> , or <code>.prjzip</code> or <code>.prj.zip</code> for zipped projects. A compressed copy of the initial state of the project is stored, if it does not already exist.
<code>-prefwarn</code>	Show warnings when preferences are read during startup.
<code>-printenv</code>	Print environment variables set during startup.
<code>-profile profile</code>	Start Maestro with the specified profile. The profile can be a custom profile, or it can be one of the standard profiles, <code>Maestro</code> , <code>BioLuminate</code> , or <code>Elements</code> . Profile names are case-sensitive, so <code>maestro</code> is not the same as <code>Maestro</code> . The default profile is used if this option is not included.
<code>-s number</code>	Specify the first structure to load when a Maestro file is loaded.
<code>-SGL</code>	Use the Schrödinger-supplied software OpenGL library. The default is to use the system (hardware) OpenGL library when displaying Maestro locally or with <code>VirtualGL</code> , and to use the software library otherwise. This option may be needed when running Maestro on a virtual machine or to diagnose or work around hardware or graphics driver issues. Linux only.
<code>-NOSGL</code>	Disable the use of the software OpenGL library and use the hardware library (even if <code>-SGL</code> is also used). Linux only.
<code>-stdtheme</code>	Use a standard theme for Maestro window decorations, panel background colors, etc., rather than the theme from the window manager. This option is useful if the window manager theme has a dark panel background, which makes the toolbar icons difficult to see.

Table 2.1. Options for the maestro command. (Continued)

Option	Description
-t <i>number</i>	Specify the total number of structures to load when a Maestro file is loaded.
-trajectory <i>CMS-file</i>	Import a Desmond structure file (.cms); if the file has an associated trajectory, load the trajectory and open the Trajectory panel. Cannot be used with other structure import options (such as -m or -b).
-u <i>menu-file</i>	Use the specified file to configure the main menu bar. You can copy a custom menu file (.mnu) from your <a href="#">Maestro user resources directory</a> .
-v	Display the Maestro version number, but do not start Maestro.

### 2.1.4 Choosing a Profile

Much of the Maestro interface can be configured or customized, through the use of preferences, toolbar, menu, and mouse customization, installation of scripts, and use of macros and shortcuts. These configuration and customization options are stored in your user profiles directory. See [Chapter 13](#) for more information on customization and the user profiles directory.

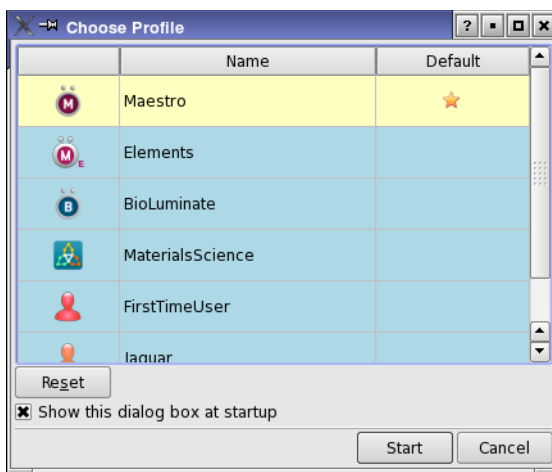
To allow the use of more than one set of customizations, Maestro supports the concept of *profiles*. A profile is a named collection of customizations and preferences that can be applied when you start Maestro. The profiles are stored in the user profiles directory, each in its own folder (subdirectory). Profile names are case-sensitive, and can include spaces and other non-alphanumeric characters. The main standard profiles are provided in the distribution:

- Maestro—for general use of Maestro.
- BioLuminate—a customization for the BioLuminate product.
- MaterialsScience—a customization for the Materials Science suite.
- Elements—a simplified Maestro interface designed for medicinal chemistry.

Some other standard profiles are available that perform different customizations, to simulate the behavior of Maestro 9.1, to simplify the interface for new users, and to emphasize small molecule features. These profiles are very similar to the main Maestro profile, except that they may have fewer menu items, or some rearrangements of the toolbars. There is no custom online help for these profiles, as there is for the main standard profiles, so you may find that documented features are not available in these profiles.

When you start Maestro without specifying a profile<sup>1</sup>, the Choose Profile dialog box opens by default. In this dialog box you can choose the profile, by selecting it from the list. To start Maestro with the chosen profile, click Start or press ENTER, or double-click on the profile you want to use.

1. Starting Maestro with a particular profile can be done from the command line or by using the icon for the profile.



**Figure 2.1.** The Choose Profile dialog box.

You can set the default profile by clicking in the Default column. If you bypass this dialog box by clearing the Show this dialog at startup option, the default profile is used to start Maestro. To return to displaying this dialog box, choose Maestro → Customize → Profiles, and select Show the Choose Profile dialog box at startup in the Customize Profiles panel. More information on customizing profiles is given in [Section 13.4 on page 319](#).

All descriptions in this manual are given for the Maestro profile.

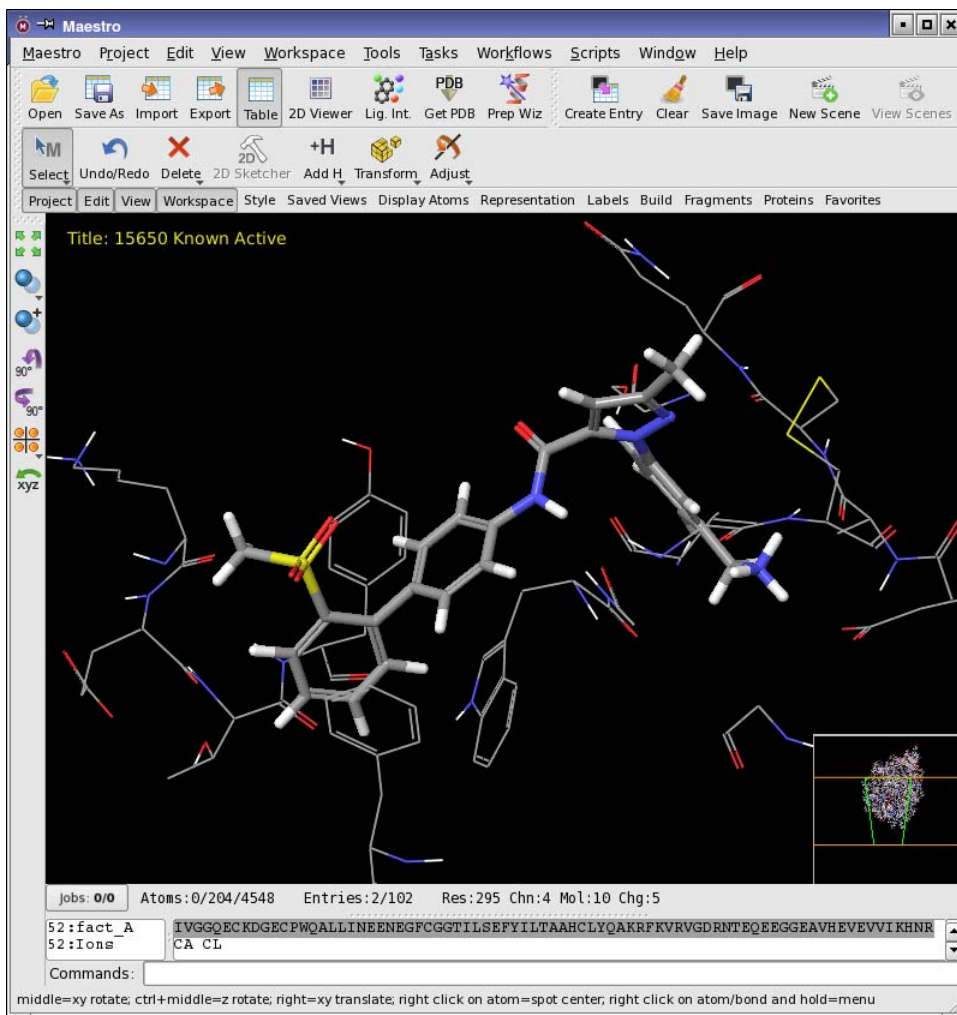
## 2.2 The Main Window

The Maestro main window is shown in [Figure 2.2](#). The following main window components are always visible:

- **Title bar**—displays the project name and the current working directory if the relevant preference is set—see [Section 14.1.4 on page 334](#).
- **Auto-Help bar**—automatically displays context-sensitive help
- **Main menu bar**—provides access to panels
- **Workspace**—displays molecular structures and other 3D graphical objects, such as surfaces and Phase hypotheses. Information on a single project entry can also be displayed in the top left corner—see [Section 14.5.2 on page 354](#).

The following main window components can be displayed or hidden by choosing the component from the Window menu. Your choice of which main window components are displayed is persistent between Maestro sessions.

- **Toolbars**—contain buttons for many common tasks. See [Section 2.4 on page 18](#) for an overview of the toolbars and references to more detailed information.
- **Status bar**—displays information about a particular atom, about structures in the Workspace, or about the contents of the Workspace and job status. See [Section 2.5 on page 24](#) for details.



**Figure 2.2.** The Maestro main window, showing all window components.

- **Clipping planes window**—displays a small, top view of the Workspace that shows the clipping planes and viewing volume indicators. Hidden by default. See [Section 4.6 on page 72](#) for details.
- **Sequence viewer**—shows sequences for proteins displayed in the Workspace. Hidden by default. See [Section 2.6 on page 26](#) for details.
- **Command input area**—provides a place to enter Maestro commands. Hidden by default. Command completion is supported for the keyword (but not the options).

When a distinction between components in the main window and those in other panels is needed, the term *main* is applied to the main window components (e.g., main menu bar).

The toolbars are dockable: they can be moved to any side of the Workspace or dragged out of the Workspace entirely.

You can expand the Workspace to occupy the full screen, by pressing CTRL+= or choosing Workspace → Full Screen. All other components and panels are hidden. To return to the previous display, press ESC.

The following sections describe some of these main window components in more detail.

## 2.3 The Menu Bar

The menus on the main menu bar provide access to panels, allow you to enter commands, and control the appearance and contents of the Workspace. The main menus are as follows:

- **Maestro**—change directories, check for software updates, set preferences, customize menus, toolbars, and mouse actions, display main window components, set up command aliases and macros, interact with PyMOL, and quit Maestro.
- **Project**—display Project Table and annotation; create, open, close, copy, delete, save, back up, restore, and merge projects; import and export structures. For more information on projects, see [Chapter 9](#).
- **Edit**—undo actions, copy and paste structures or images, delete Workspace objects, select atoms, find atoms, build and modify structures, and mark entries.
- **View**—change the view of the Workspace objects (rotate, translate, zoom, align) or the view attributes (clipping, perspective, depth perception, fog), enter or exit stereo mode, save or restore particular views, tile the Workspace.
- **Workspace**—control the display of the contents of the Workspace, save Workspace images and Workspace “scenes”.

- **Tools**—group atoms; measure, align, superimpose, and minimize structures; assign structural features; and view and visualize data.
- **Applications**—set up, submit, and monitor jobs for Schrödinger’s computational programs. Some products have a submenu from which you can choose a specific task.
- **Tasks**—Run various tasks. Alternative to Applications menus.
- **Workflows**—set up, submit, and monitor jobs for KNIME workflows.
- **Scripts**—manage, install, and run scripts. For details, see [Section 15.1 on page 377](#).
- **Window**—close or reopen all panel, arrange panels in a cascade, save or load a panel layout, raise individual or all open panels.
- **Help**—display various kinds of documentation, including online help, manuals, information about Maestro and other Schrödinger products.

The functions of the items on the menus are described in detail in later chapters of this manual. The menus and items as described here are the Maestro defaults. You can customize the menus by adding or removing items, changing the names, keyboard shortcuts, and mnemonics—see [Section 13.2 on page 314](#). If you do, the descriptions of the locations given in this manual do not, of course, apply to the changed items.

## 2.4 The Main Window Toolbars

The main window has a number of toolbars, which allow you to perform many of the common tasks. Each toolbar contains buttons for a particular kind of task.

The toolbars contain three kinds of buttons for performing common tasks:



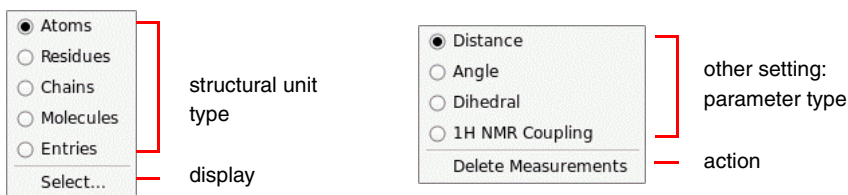
**Action**—Perform a simple task, like clearing the Workspace.



**Display**—Open or close a panel or open a dialog box, such as the Project Table panel.



**Menu**—Display a *button menu*. These buttons have a triangle in the lower right corner.



**Figure 2.3. Examples of button menus.**

There are five types of items on button menus, and all four types can be on the same menu (see [Figure 2.3](#)):

- **Action**—Perform an action immediately.
- **Display**—Open a panel or dialog box.
- **Structural unit for picking**—Choose Atoms, Bonds, Residues, Chains, Molecules, or Entries, then click on an atom in the Workspace to perform the action on all the atoms in that structural unit. The structural unit types are included as radio buttons on the menu, and the button is highlighted to indicate that this is the action to be performed.
- **Atom category for selection**—Choose one of a list of categories of atom to apply the action to all atoms of this type in the Workspace. The list of categories is the same as on the Select button (though with slightly different wording)—see [Section 6.2 on page 119](#).
- **Other setting**—Set a state, choose an attribute, or choose a parameter type and click on atoms in the Workspace to act upon that parameter.

The toolbar buttons can be displayed as an icon, as text, or as both. The choice can be made for each toolbar separately, by right clicking on the toolbar and choosing an option from the Style submenu of the shortcut menu. You can also change the style for all toolbars in the Preferences panel, under General → Appearance, where you can also change the font for the toolbar buttons—see [Section 14.1.4 on page 334](#).

The choice of buttons that appears on each toolbar can be customized, by choosing Maestro → Customize → Toolbars, or choosing Customize from the toolbar shortcut menu. The Customize Toolbars panel has a menu of toolbars at the top, a list of all available buttons on the left, categorized by function, and a list of buttons that are on the selected toolbar on the right. You can choose buttons from any of the categories and add them to any toolbar. You can also create your own toolbar, by clicking New, naming the toolbar, and adding the desired buttons. A toolbar named Favorites has been included for you to customize; by default it has no buttons.

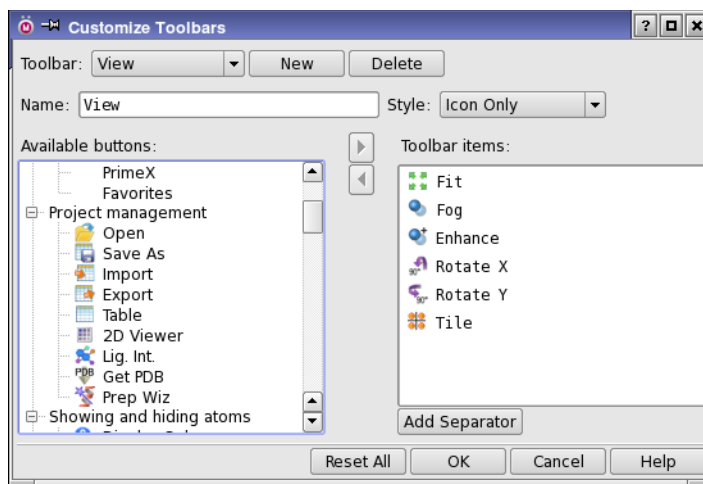


Figure 2.4. The Customize Toolbars panel.

As well as adding toolbars, you can delete toolbars, including the predefined toolbars. To do so, choose the toolbar from the Toolbar option menu, and click Delete. As the customizations are stored in your profile, you can always restore toolbars from the installation.

To reset all toolbars to their defaults, click Reset All.

The complete list of main window toolbars is:

- **Manager toolbar**—contains buttons for showing or hiding the other toolbars. You can also show and hide toolbars with Window → Toolbar.
- **Project toolbar**—contains buttons for common project-related tasks. This toolbar is described below.
- **Edit toolbar**—contains buttons for atom selection and editing structures, in addition to the usual Undo/Redo, Cut, Copy, Paste, and Delete buttons. This toolbar is described below.
- **View toolbar**—contains buttons for changing the view of the Workspace. See [Section 4.1 on page 63](#) for details.
- **Workspace toolbar**—contains buttons for common Workspace operations and for scenes. This toolbar is described below.
- **Style toolbar**—contains buttons for setting the visual style of the contents of the Workspace, including representation, color scheme, ribbons, atom display, surfaces. See [Section 7.6 on page 153](#) for details.



- **Saved Views toolbar**—contains buttons for saving, restoring, and managing views. See [Section 4.3 on page 67](#) for details.
- **Display Atoms toolbar**—contains buttons for displaying and undisplaying atoms. See [Section 7.5 on page 149](#) for details.
- **Representation toolbar**—contains buttons for changing the molecular representation and ribbons. See [Section 7.1 on page 133](#) for details.
- **Labels toolbar**—contains buttons for various annotations in the Workspace, including atom labels, captions, highlights, and single-entry feedback. See [Section 8.1 on page 161](#) for details.
- **Build toolbar**—contains buttons for various structure-building tasks. See [Section 5.1 on page 79](#) for details.
- **Fragments toolbar**—contains a small selection of molecular fragments for building. See [Section 5.1 on page 79](#) for details.
- **Find toolbar**—contains tools for finding various structural objects in the Workspace. See [Section 2.10 on page 37](#) for details.
- **Proteins toolbar**—contains buttons for various protein-related tasks. See [Section 3.7](#) of the *PrimeX User Manual* for details.
- **Periodicity toolbar**—contains buttons for display of periodic structures. [Section 7.5.3 on page 152](#) for details.
- **Favorites toolbar**—contains no buttons by default, but is intended for you to customize.

The toolbar buttons for the default Project, Edit, and Workspace toolbars are described below. Many of their features are described in later chapters.

### 2.4.1 The Project Toolbar

This toolbar contains buttons for the common project operations.



#### Open

Open a project. Opens the Open Project project selector so you can select a project to open.  
Menu equivalent: Project → Open.



#### Save As

Save a project by a different name.  
Menu equivalent: Project → Save As.



#### Import

Import structures into the project as new entries. Opens the Import panel.  
Menu equivalent: Project → Import Structures.



### Export

Export structures from the project to file. Opens the Export dialog box.  
Menu equivalent: Project → Export Structures.



### Table

Open or close the Project Table panel.  
Menu equivalent: Project → Show Table.



### 2D Viewer

Display 2D structures of the selected entries in a grid. Opens the 2D Viewer panel.  
Menu equivalent: Project → 2D Viewer.



### Lig. Int.

Display a simplified representation of ligand-receptor interactions. Opens the Ligand Interaction Diagram panel.  
Menu equivalent: Tools → Ligand Interaction Diagram.



### Get PDB

Retrieve a structure from the PDB and import it into the project. Opens the Get PDB File dialog box.  
Menu equivalent: Project → Get PDB.



### Prep Wiz

Prepare a protein for use in calculations. Opens the Protein Preparation Wizard panel.  
Menu equivalent: Workflows → Protein Preparation Wizard.

## 2.4.2 The Edit Toolbar

This toolbar contains buttons for atom selection and editing structures, in addition to the usual buttons found on Edit toolbars.



### Select

Select atoms in the Workspace. Double-click to select all atoms.  
This button has a menu from which you can choose the type of structural unit you want to select. If you select a structural unit from the menu, the icon changes to reflect that structural unit (A for atoms, R for residues, etc.). You can expand the selection to include entire residues within a specified distance by choosing one of the distance options, and you can include or exclude the picked object in the final selection.  
You can choose Select to open the Atom Selection dialog box and specify atoms to select.  
Menu equivalent: Edit → Select Atoms.



### Undo/Redo

Undo or redo the last action. The button icon and text changes, depending on the action.  
Menu equivalent: Edit → Undo/Redo.



### Cut

Delete the selected atoms from the Workspace and place them on the clipboard, in Maestro format and in SMILES format.  
Menu equivalent: Edit → Cut.

**Copy**

Copy the selected atoms and an image of the Workspace onto the clipboard. The selected atoms are stored in Maestro and SMILES format. The resolution of the image is the current screen resolution, so if you want a higher resolution, you should use the **Save Image** panel. Menu equivalent: **Edit** → **Copy**.

**Paste**

Paste a structure from the clipboard into the Workspace. The structure can be a SMILES string, a structure from ChemDraw or Isis Draw (Windows) or a set of atoms previously cut or copied from the Workspace.

SMILES strings are converted into 2D structures, and added to the project as a new entries, with the SMILES string as the title. No attempt is made at 3D conversion. To paste it in 3D, choose **Edit** → **Paste Special** → **As 3D**.

Atoms that were cut or copied from Maestro are placed at the coordinates at which they were cut or copied onto the clipboard, as a scratch entry. You can paste atoms from one Maestro session into another session.

Menu equivalent: **Edit** → **Paste**.

**Delete**

Delete objects in the Workspace. The button menu has several sections: one for the current selection (**DELETE**), one for structural units to pick for deletion, one for other kinds of structural objects to delete, and one for markers and annotations. Double-click to delete the selected atoms.

Menu equivalent: **Edit** → **Delete** → **Pick to Delete**.

**Build**

Show or hide the **Build** toolbar and **Fragments** toolbar, or open the **Build** panel from the menu. Menu equivalent: **Edit** → **Build**.

**2D Sketcher**

Sketch to edit or create structures in 2D. Opens the **2D Sketcher** panel.

Menu equivalent: **Edit** → **2D Sketcher**.

**Add H**

Add hydrogen atoms to a structure that lacks them, to complete the valence. From the button menu you can choose the type of structural unit to pick for addition of hydrogens, open the **Atom Selection** dialog box to select the atoms, or choose a hydrogen treatment. Double-click to add hydrogens to the selected atoms.

Menu equivalent: **Edit** → **Add Hydrogens**.

**Transform**

Transform (rotate or translate) selected atoms in the Workspace. From the button menu you can choose to display hydrogen bonds, contacts, and bond lengths while transforming, choose a structural unit to pick the atoms to transform, or open the **Advanced Transformations** panel for more control over the transformation.

Menu equivalent: **Edit** → **Transform**.

**Adjust**

Adjust the geometry of structures. From the button menu you can choose geometric parameters to adjust: distances, angles, dihedrals or chirality; torsions, peptides, or side chains (rotamers); or choose to display hydrogen bonds and contacts while adjusting torsions.

Menu equivalent: **Edit** → **Adjust**.

### 2.4.3 The Workspace Toolbar

This toolbar contains buttons for some common Workspace operations, and buttons for creating and managing scenes.



#### Create Entry

Create an entry in the current project using the contents of the Workspace. Opens a dialog box in which you can supply a title for the entry, and choose whether to create the entry from all atoms, the selected atoms, or the displayed atoms. If all the atoms in the new entry come from entries in the same entry group, the new entry is added to the same group, otherwise it is added to the ungrouped entries in the Project Table.

Menu equivalent: Workspace → Create Project Entry.



#### Clear

Clear the Workspace. Excludes all entries in the Project Table, and deletes the contents of the scratch entry, if there is one.

Menu equivalent: Workspace → Clear.



#### Save Image

Save an image of the Workspace to a file in TIFF, JPEG, or PNG format, in the Save Image panel.

Menu equivalent: Workspace → Save Image.



#### New Scene

Create a new “scene”, which is a snapshot of part or all of the project, including the Workspace content and display settings. Opens the New Scene dialog box, in which you can provide a description and choose which parts of the project to include in the scene.

Menu equivalent: Workspace → Scenes → New.



#### View Scenes

Enter a mode in which you view scenes. The Scenes toolbar is displayed in a bar at the bottom of the Workspace, and the selected scene is opened. While you are viewing scenes, no changes are made to the project.

Menu equivalent: Workspace → Scenes → View.

## 2.5 The Status Bar

The status bar displays information about the contents of the Workspace or about a particular atom, depending on where the pointer pauses. If the pointer is not over an atom, information about the contents of the Workspace is displayed, in the format

```
Atoms:sa/ma/na Entries:me/ne Res:nr Chn:nc Mol:nm Chg:n
```

where the fields in the display have the following meanings:

---

Atoms	Number of atoms in the Workspace: <i>sa</i> is the number selected, <i>ma</i> is the number displayed, <i>na</i> is the total
Entries	Number of entries in the Workspace: <i>me</i> is the number displayed, <i>ne</i> is the total
Res	Number of residues <i>nr</i> in the Workspace
Chn	Number of chains <i>nc</i> in the Workspace
Mol	Number of molecules <i>nm</i> in the Workspace
Chg	Total charge <i>n</i> of the Workspace contents

If the pointer is over an atom, and the preference to show feedback on atoms is set, the status bar displays the chain, residue number, element, PDB atom name, formal charge, and a user-selected property, in the format

*atom:chain:residue number : (element) PDB :charge: "userchoice"*

where the fields in the display have the following meanings:

<i>atom</i>	Atom number in the Workspace
<i>chain</i>	Chain name
<i>residue</i>	Residue name
<i>number</i>	Residue number and insertion code
<i>element</i>	Element
<i>PDB</i>	PDB atom name
<i>charge</i>	Formal charge of the atom
<i>userchoice</i>	Selected Project Table property

If you are picking an object in the Workspace and you have the preference set, the index of the object is displayed at the beginning of the status bar, in the format `Pick: index`. For example, if you are picking molecules, the molecule number is displayed.

The preferences to show feedback and the user-selected property can be set under Feedback – Atoms in the Preferences panel—see [Section 14.5.1 on page 354](#).

On the left of the status bar is a button that displays job status information. The text on the button gives the number of jobs in the format `Jobs: mj/nj`, where *mj* is the number in the project and *nj* is the total number. Clicking the button opens the Monitor panel. The tool tip for the button displays information on the status of the first few jobs in the Monitor panel.

## 2.6 The Sequence Viewer

The sequence viewer displays the sequence of the proteins that are included in the Workspace. Each chain is displayed on a separate line. If the sequence is longer than a single line, the entire set of lines is continued below the first set of lines (“wrapped”) by default. The left column of the sequence viewer displays a label for the sequence, in the format *row: pdbID\_chainID*, where *row* is the Project Table row number. The right column displays the actual sequence as a list of single-letter codes, and also displays the secondary structure assignment, if one is available.

The background colors of the sequences reflect the current coloring scheme for the alpha carbon in the Workspace. Each residue in the sequence also has a tooltip that gives the residue name, number, and insertion code.

If the protein has a secondary structure assignment, the assignment is displayed above the sequence, using the following symbols:

- Helices are displayed as tubes, colored red
- Strands are displayed as arrows, colored cyan
- Loops are displayed as a gray line.

You can select residues in the sequence and perform actions on these residues.

- To select a single residue, click the residue.
- To add single residues to the selection or remove single residues from the selection, control-click the residues.
- To select a range of residues, click the first and shift-click the last, or drag over the residues. If the sequence viewer is wrapped, you can drag over multiple rows to select residues in more than one row (but only in the sequence in which you started dragging).
- To change the selection of a contiguous set of residues, hold down the CTRL key and drag over the set of residues. The unselected residues are selected, and the selected residues are deselected. This can be used to extend the selection or add a discontinuous sequence fragment to the selection, for example.

The selected residues are highlighted in reverse video (as colored letters on a black background), and are marked in yellow in the Workspace.

The sequence viewer and the Workspace are synchronized: selection of atoms in the Workspace selects the corresponding atoms in the sequence viewer, and selection of residues in the sequence viewer selects them in the Workspace. Likewise, changing the color scheme in the Workspace changes the color scheme in the sequence viewer, and vice versa. Structural changes, such as mutating a residue, are also reflected in the sequence viewer.

To zoom in on a residue in the Workspace without selecting it, middle-click the residue in the sequence viewer.

The sequence viewer has a shortcut menu (right-click and hold), which you can use to perform various actions on the sequences or the display. If you do not have any residues selected in the sequence viewer, the sequence viewer shortcut menu is displayed. The items on this menu are described in [Table 2.6](#). If you have residues selected, the selection shortcut menu is displayed (see [Table 2.3](#)). In this context there is one extra item on the Color Scheme submenu: Proximity. If you choose this item, the residues within a given distance of the selected residues are colored orange, and the selected residues are colored red. All others are colored gray. To remove this color scheme, deselect the residues and choose None from the Color Scheme submenu. The distance is specified in the Sequence Viewer - Preferences dialog box, which you open from the sequence viewer shortcut menu.

## 2.7 Shortcut Menus

Some of the main window components have shortcut menus, which you open by right-clicking and holding over the component.

The status bar, the toolbars, and the command input area have two common items, Hide, which hides the component, and Help, which displays the relevant help topic. These are the only items for the status bar.

The toolbars have a Customize item to open the Customize Toolbars panel for customization—see [Section 2.4 on page 18](#). The toolbars other than the Manager toolbar have a Style item, from which you can select the arrangement and appearance of the icon and the text for the buttons.

The command input area has a standard set of text input items, which are described in [Section 1.1.3 on page 3](#).

The Workspace has three shortcut menus: one for the Workspace itself (the *Workspace shortcut menu*), one for the atoms in the current selection (the *selection shortcut menu*), and one for bonds (the *bond shortcut menu*). The selection shortcut menu is also available from the sequence viewer. These shortcut menus have common items for tiling when used in the Workspace. The items on these menus are described in [Table 2.2](#), [Table 2.3](#), [Table 2.4](#), and [Table 2.5](#). The differences in the selection shortcut menu between the Workspace and the sequence viewer are noted in the table.

The sequence viewer has a shortcut menu for the sequence label area, which is described in [Table 2.6](#). This is in addition to the selection shortcut menu, which is displayed when you right-click on a sequence.

When you right-click and hold in the Workspace:

- On an unselected atom, the atom becomes the selection and the selection shortcut menu is displayed.
- On a selected atom, the selection shortcut menu is displayed.
- On a bond, the two atoms in the bond become the selection and the bond shortcut menu is displayed.
- On empty space, if there is an atom selection, the selection shortcut menu is displayed, otherwise the Workspace shortcut menu is displayed.

*Table 2.2. Workspace shortcut menu items.*

<b>Menu Item</b>	<b>Action</b>
Background Color	Set the Workspace background color to black, white, gray, or blue.
Workspace Feedback	Set up entry properties to be shown at the top left of the Workspace (“feedback”). Opens the Preferences panel at the Feedback – Entry section.
Save Image	Open the Save Image panel to save an image of the Workspace in TIFF, JPEG, or PNG format.
Save View	Save the current view of the Workspace (orientation, location, and zoom).
Restore View	Restore the last saved view of the Workspace (orientation, location, and zoom).
Manage Views	Open the Manage Views panel to work with the saved Workspace views.
Fit to Workspace	Fit the displayed structure to the Workspace and reset the center of rotation.
Create Project Entry	Create a Project Table entry from the Workspace.
Clear Workspace	Clear the Workspace.
Delete	Delete labels, measurements, or adjustments.
Highlights	Add or change highlights on the Workspace structures.
Caption	Add captions to the Workspace, delete captions or edit captions.
Help	Open the Shortcut Menus help topic.



Table 2.3. Selection shortcut menu items.

Menu Item	Action
Background Color	Set the Workspace background color to black, white, gray, or blue.
Workspace Feedback	Set up entry properties to be shown at the top left of the Workspace (“feedback”). Opens the Preferences panel at the Feedback – Entry section.
Invert Selection	Select the unselected atoms and deselect the selected atoms.
Expand Selection	Expand the selection to include atoms or residues within a specified distance, or to select only these atoms. (Workspace only).
Select Matching Atoms By	Select all atoms that match any of the currently selected atoms by Color, Representation, or Element (which you choose from the submenu). For example, if the selection has red and green atoms, all red and green atoms are selected.
Representation	Set the molecular representation to wire frame, ball and stick, CPK, tube, or thin tube.
Color Scheme	Apply the color scheme from the submenu to the selected atoms.
Labels	Apply the label from the submenu to the selected atoms.
Highlights	Add a highlight of a particular type with the default settings or manage highlights. (Workspace only).
Display	Display the entire molecules or residues containing the selected atoms. This action is useful if part of the molecule or residue was previously undisplayed. Also, display residues within a given distance of the selected atoms.
Display Only	Display only the selected atoms. (Workspace only).
Undisplay	Undisplay the selected atoms.
Delete	Delete the selected atoms.
Switch Alternate Positions	For atoms with partial occupancy, switch between the alternate positions. (Workspace only.)
Display Alternate Positions	For atoms with partial occupancy, display all positions. The alternate positions are displayed as ghosts. (Workspace only.)
Set Element	Change the selected atoms to atoms of the element chosen from the submenu. (Workspace only.)
Insert Gap	Insert a gap to the left of the selected residue. Opens a dialog box in which you can specify the number of residues to insert. (Sequence viewer only.)
Mutate Residue	Change the residues that contain the selected atoms (or the selected residues) to the type chosen from the submenu.
Rotamers	Open the Rotamers dialog box to select one of the standard rotamers for the selected residues.

*Table 2.3. Selection shortcut menu items. (Continued)*

<b>Menu Item</b>	<b>Action</b>
Create Project Entry	Create a project entry. Opens the Create Project Entry dialog box, in which you can provide a title for the entry, and choose whether to use the selected atoms, the displayed atoms, or all atoms. (Workspace only.)
Exclude Entries	Exclude the entries that contain the selected atoms from the Workspace.
Select Project Entries	Select the entries that contain the selected atoms in the Project Table. The submenu allows you to choose whether to add the entries to the current Project Table selection, or to replace the selection.
Fit to Workspace	Fit the displayed structure to the Workspace and reset the center of rotation.
Clip	Clip the display to the selected atoms. Moves the clipping planes. (Workspace only.)
Center Electron Density	Center the displayed electron density map on the centroid of the selected atoms. Used for PrimeX. (Workspace only.)
Transform	Perform a local transformation. (Workspace only.)
Align Centers of Mass	Translate the entries so that the centers of mass of the selected atoms in each entry coincide. (Workspace only.)
Help	Open the Shortcut Menus help topic.

*Table 2.4. Bond shortcut menu items.*

<b>Menu Item</b>	<b>Action</b>
Order	Set the bond order to zero, one, two, or three.
Measure	Measure the bond length and display it. The measurement is added to the list in the Measurements panel.
Adjust	Adjust the bond length or the dihedral angle around this bond.
Delete	Delete the bond.

*Table 2.5. Tiling items on shortcut menus.*

<b>Menu Item</b>	<b>Action</b>
Apply Zoom to All Tiles	Apply the zoom value from the current tile to all tiles.
Apply View to All Tiles	Apply the view (rotation, translation, zoom) from the current tile to all tiles.
Reset Tile	Reset the view of the current tile to its initial value.
Pick Tiles to Move	Turn on or off picking to move tiles. When enabled, picking selects tiles which can then be moved to a new location.

Table 2.6. Sequence viewer shortcut menu items.

Menu Item	Action
Hide	Hides the sequence viewer. To redisplay it, use the Window menu.
Color Scheme	Colors the sequence with the scheme selected from the submenu. Choose from None, Color by Chain, Residue Type, Residue Property, Secondary Structure, Template ID, or Proximity (sequence viewer only).
Font Size	Sets the font size for the sequence viewer. Choose Small, Medium, Large, or Huge from the submenu.
View SSA	Shows or hides the secondary structure assignment for the sequence.
Show Displayed Residues Only	Shows only the residues that are displayed in the Workspace.
Display Non-protein Molecules	Display non-protein molecules in the sequence viewer. Three lines are used, for ligands, waters, and ions.
Align by Residue Number	Aligns the sequences in the sequence viewer by residue number. (Does not affect the alignment of the structures.) This command enables gaps to be displayed in the sequence viewer.
Exclude Entry	Excludes the entry containing this chain from the Workspace. The chain is removed from the sequence viewer. If the entry contains multiple chains, all the chains in the entry are removed from the sequence viewer.
Wrap Sequences	Wraps the sequence display so that long sequences are displayed across multiple lines with vertical scrolling rather than on a single line with horizontal scrolling.
Legend	Opens the Sequence Viewer Legend dialog box, which explains the sequence color schemes.
Preferences	Opens the Sequence Viewer - Preferences dialog box, in which you can set the proximity cutoff.
Save Image	Opens the Save Sequence Viewer Image file selector, in which you can save an image of the sequence viewer to a file. The image format is determined by the extension that you choose.
Export Sequences	Exports the sequences in the Sequence Viewer to a FASTA file. Opens a file selector to specify the location and the file name.
Help	Opens the Sequence Viewer help topic.

## 2.8 Mouse Functions

The Workspace has special uses for the middle and right mouse buttons. These are used on their own and in combination with the SHIFT and CTRL keys to perform common operations such as rotation, translation, centering, and zooming. The table below summarizes the standard actions for a 3-button mouse with scroll wheel.

Table 2.7. Mapping of Workspace operations to mouse actions.

Mouse Button	Keyboard	Motion	Action
Left		click, drag	Select
Left		drag	Quick Torsion adjustment and adjustment of distance, angle, dihedral
Left	SHIFT	click, drag	Toggle the selection
Middle		drag	Rotate about X and Y axes
Middle	SHIFT	drag vertically	Rotate about X axis
Middle	SHIFT	drag horizontally	Rotate about Y axis
Middle	CTRL	drag horizontally	Rotate about Z axis
Middle	SHIFT + CTRL	drag horizontally	Zoom
Right		click	Spot-center on selection Toggle selection
Right		click and hold	Display shortcut menu
Right		drag	Translate in the X-Y plane
Right	SHIFT	drag vertically	Translate along the X axis
Right	SHIFT	drag horizontally	Translate along the Y axis
Right	CTRL	drag horizontally	Translate along the Z axis
Middle & Right		drag horizontally	Zoom
Wheel		scroll	Zoom In any adjust mode, do adjustment
Wheel	CTRL	scroll	Adjust isovalue of electron density map (PrimeX) In clipping planes window, move clipping planes in opposite directions
Wheel	SHIFT	scroll	In clipping planes window, move clipping planes in the same direction

Section 4.2 on page 64 has more detailed information on changing the Workspace view. Mouse and trackpad functions can be customized—see Section 13.3 on page 317 for information

## 2.9 Shortcut Keys

Some frequently used operations in the main window have been assigned shortcut key combinations. The default shortcuts, their functions, and their menu equivalents are listed in Table 2.8. Shortcut keys in the Project Table panel and the Plot panel are listed in the chapters that describe those panels. In addition to the shortcut keys listed below, there are a set of keys that can be used in either the Workspace or the Project Table. Most of these keys are for actions in the Project Table—see Section 9.4.6 on page 192 for more information. You can customize the shortcut keys in the Customize Menus panel—see Section 13.2 on page 314 for details.

If Num Lock, Caps Lock, or Scroll Lock is enabled, the shortcut keys do not work. Some shortcut keys might not work on non-English keyboards: for example, CTRL+= (full screen) on German keyboards in the German locale or ` (pick to select) on French keyboards in the French locale. If this is the case, you can customize the shortcut keys for these functions.

Table 2.8. Default shortcut keys in the Maestro main window.

Keys	Action	Equivalent Menu Choice
B	Pick bonds in the Workspace	
CTRL+SHIFT+Z (⇧⌘Z)	Select the next defined adjustment of the current type for adjustment.	Edit → Adjust → Next Adjustment
CTRL+SHIFT+A (⇧⌘A)	Select the previous defined adjustment of the current type for adjustment.	Edit → Adjust → Previous Adjustment
U	Clean up the geometry of the Workspace structure or selected atoms.	Edit → Build → Clean Up Geometry
CTRL+C (⌘C)	Copy the Workspace contents onto the clipboard. Includes atoms, SMILES, and image at screen resolution.	Edit → Copy
CTRL+X (⌘X)	Cut the atom selection (delete the selected atoms and put them on the clipboard)	Edit → Cut
DEL	Delete the selected atoms	Edit → Delete
CTRL+F (⌘F)	Show or hide the Find toolbar	Edit → Find
X	Mark or clear mark for the current entry, creating the Mark property if necessary.	Edit → Mark Target Entry
CTRL+V (⌘V)	Paste atoms into the scratch entry	Edit → Paste

Table 2.8. Default shortcut keys in the Maestro main window. (Continued)

Keys	Action	Equivalent Menu Choice
CTRL+SHIFT+V (⇧⌘V)	Paste atoms into the scratch entry so that the centroid is at the picked location.	Edit → Paste Special → By Placing
A	Pick atoms in the Workspace for the current action.	Edit → Pick → Atoms
C	Pick chains in the Workspace for the current action.	Edit → Pick → Chains
E	Pick entries in the Workspace for the current action.	Edit → Pick → Entries
M	Pick molecules in the Workspace for the current action.	Edit → Pick → Molecules
R	Pick residues in the Workspace for the current action.	Edit → Pick → Residues
CTRL+A (⌘A)	Select all atoms	Edit → Select Atoms → All
N	Select the next residue in the structure from the currently selected residue.	Edit → Select Atoms → Next Residue
`	Select atoms by picking.	Edit → Select Atoms → Pick to Select
P	Select the previous residue in the structure from the currently selected residue.	Edit → Select Atoms → Previous Residue
1, 2, ..., 0	Select atoms in previously saved atom set 1, 2, ..., 10.	Edit → Select Atoms → Restore → Atom Set <i>n</i>
CTRL+1 (⌘1), CTRL+2 (⌘2), ... CTRL+0 (⌘0)	Save the selected atoms as atom set 1, 2, ..., 10.	Edit → Select Atoms → Save → Atom Set <i>n</i>
*	Cycle through number of stars assigned to the target entry, in increasing order.	Edit → Star Target Entry
CTRL+G (⌘G)	Enter and exit local transformation mode	Edit → Transform → Pick to Transform
CTRL+Z (⌘Z)	Undo/Redo the last command.	Edit → Undo/Redo
CTRL+H (⌘H)	Display the default help topic	Help → Online Help
CTRL+, (⌘,)	Open the Preferences panel	Maestro → Preferences
CTRL+Q (⌘Q)	Quit Maestro	Maestro → Quit
CTRL+W (⌘W)	Close the project.	Project → Close

Table 2.8. Default shortcut keys in the Maestro main window. (Continued)

Keys	Action	Equivalent Menu Choice
CTRL+E (⌘E)	Open the Entry List panel	Project → Entry List
CTRL+I (⌘I)	Open the Import panel	Project → Import Structures
CTRL+N (⌘N)	Create a new project	Project → New Project
CTRL+O (⌘O)	Open an existing project	Project → Open Project
CTRL+T (⌘T)	Open the Project Table panel	Project → Project Table
CTRL+R (⌘R)	Open the Task Tree panel	Tasks → Show Tree
CTRL+M (⌘M)	Minimize the selected atoms (or all atoms, if there is no selection)	Tools → Minimize → Selected Atoms
CTRL+SHIFT+M (⇧⌘M)	Minimize the ligand.	Tools → Minimize → Ligand
D	Turn on and off enhancement of depth view with ambient spherical occlusion.	View → Enhanced Depth View
L	Fit the ligand to the Workspace. If there is more than one ligand-sized molecule, cycle through them with repeated use of L.	View → Fit to Workspace → Ligand
Z	Fit the selected atoms or all atoms to the Workspace	View → Fit to Workspace → Selected Atoms
G	Move clipping planes further apart	View → Move Clipping Planes → Apart
–	Move clipping planes back (away from user)	View → Move Clipping Planes → Back
=	Move clipping planes forward (toward user)	View → Move Clipping Planes → Forward
F	Move clipping planes closer together	View → Move Clipping Planes → Together
;	Rotate the view in the positive x direction by the keyboard rotation increment.	View → Rotate → +X
/	Rotate the view in the negative x direction by the keyboard rotation increment.	View → Rotate → -X
.	Rotate the view in the positive y direction by the keyboard rotation increment.	View → Rotate → +Y
,	Rotate the view in the negative y direction by the keyboard rotation increment.	View → Rotate → -Y

*Table 2.8. Default shortcut keys in the Maestro main window. (Continued)*

<b>Keys</b>	<b>Action</b>	<b>Equivalent Menu Choice</b>
]	Rotate the view in the positive z direction by the keyboard rotation increment.	View → Rotate → +Z
[	Rotate the view in the negative z direction by the keyboard rotation increment.	View → Rotate → -Z
:	Translate the view in the positive x direction by the keyboard translation increment.	View → Translate → +X
?	Translate the view in the negative x direction by the keyboard translation increment.	View → Translate → -X
>	Translate the view in the positive y direction by the keyboard translation increment.	View → Translate → +Y
<	Translate the view in the negative y direction by the keyboard translation increment.	View → Translate → -Y
}	Translate the view in the positive z direction by the keyboard translation increment.	View → Translate → +Z
{	Translate the view in the negative z direction by the keyboard translation increment.	View → Translate → -Z
Y	Enter and exit rotation mode, in which the use of the mouse for picking is suspended and mouse actions perform rotation of the view.	View → Transform Mode → Rotation
CTRL+S (⌘S)	Enter and exit stereo viewing mode	View → Stereo
CTRL+L (⌘L)	Tile the Workspace by entry	View → Tile → Tile Workspace
CTRL+SHIFT+L (⇧⌘L)	Switch between transforming all tiles and transforming a single tile	View → Tile → Transform All Tiles
K	Zoom in. Same as one click on the scroll wheel.	View → Zoom In
J	Zoom out. Same as one click on the scroll wheel.	View → Zoom Out
CTRL+SHIFT+I (⇧⌘I)	Show or hide the Command Input Area.	Window → Command Input Area
CTRL+D (⌘D)	Open the Command Script Editor panel	Window → Command Script Editor
CTRL+SHIFT+N (⇧⌘N)	Create a project entry from the structures in the Workspace	Workspace → Create Project Entry



Table 2.8. Default shortcut keys in the Maestro main window. (Continued)

Keys	Action	Equivalent Menu Choice
CTRL+= (⌘=)	Enter full screen mode (Workspace occupies full screen)	Workspace → Full Screen
CTRL+> (⌘>)	Open and display the next scene.	Workspace → Scene → Next Scene
CTRL+< (⌘<)	Open and display the previous scene.	Workspace → Scene → Previous Scene
S	Display or undisplay entry information in the Workspace (subject to a preference).	Workspace → Single-Entry Feedback
CTRL+Y (⌘Y)	Apply the Workspace style.	Workspace → Style → Apply Style

## 2.10 Finding Objects in the Workspace

If you want to find an atom, residue, or other group of atoms in the Workspace, you can do so with the Find toolbar, which you display by pressing CTRL+F (⌘F), choosing Edit → Find, or choosing Windows → Toolbars → Find.

To search for a particular kind of object, choose the object from the Find option menu. For each of the menu choices, the toolbar is configured so you can define the object (atoms) to search for. When you have defined the object, press ENTER to run the search, or click N or P.

- **Residue number**—Enter the residue number in the text box. You can also specify the chain name and insertion code, e.g. A:15B, but these are optional. If the chain name is not specified, all the residues with the specified residue number (and insertion code if specified) are found. If the insertion code is not specified, all the residues with the specified residue number (and PDB chain name if specified) are found.
- **Atom number**—Enter the atom number in the text box. Since atom numbers are unique, this search finds only one atom. Press ENTER to find the atom.
- **SMARTS**—Enter the SMARTS expression into the text box, or select atoms in the Workspace and click Get from Selection to generate the SMARTS expression for those atoms. (You can set preferences for some of the notational elements in the generated SMARTS pattern—see [Section 14.14 on page 375](#).) You can copy a SMARTS pattern from another location and paste it in with CTRL+V.
- **Residue type**—Choose a residue type from the option menu. This menu includes only the residues that are present in the Workspace.

- Secondary structure—Choose a secondary structure element from the option menu, from Helix, Loop, or Strand.
- Element—Enter a standard element symbol in the text box, e.g. Cl.
- PDB atom name—Enter a standard PDB atom name in the text box, e.g. CA. Spaces are significant, as 'CA ' and ' CA ' are not the same.
- Specified atoms—Enter an ASL expression in the text box, or click Select to open the Atom Selection dialog box and make an atom selection. This tool can be used to find objects that are not on the menu. For example, to find molecule number 3, enter mol.num 3 in the text box.

When you do the search, all instances of the object that match are located. The number of matched objects and the index of the current matched object is shown in a text area. You can step through the instances with the N (next) and P (previous) buttons. The instance of the object that you step to becomes the Workspace selection. If you want to fit the object to the Workspace, select Fit.

If there is only one match, the N and P buttons are disabled after the match is found. In this case, if you want to find the match again, click in the text box and press ENTER. These buttons are always disabled for Atom number, so you must press ENTER to find an atom by number.

If you have a single residue selected, you can step through the residues in sequence by pressing the N or P keys. If you reach the end of the chain, the next residue found is the lowest residue in the next chain or the highest residue in the previous chain.

## 2.11 Undoing Workspace Operations

Single operations in the Workspace can be undone by choosing Undo *action* from the Edit menu. This item is dynamic: its name includes a description of the last undoable action, and changes to Redo after it has been used. Selecting Redo *action* reimplements the action that was undone. This menu item is mapped to the Undo/Redo button on the toolbar.

**To undo the last operation, do one of the following:**

- Click the Undo/Redo button on the toolbar.



- Choose Undo *action* from the Edit menu.
- Press CTRL+Z.

If you want to be able to undo more than one operation, you can define an Undo block. The Undo block groups a sequence of commands so that the effect of the entire sequence can be reversed. This is particularly useful for risky or complicated procedures.

**To define an Undo block:**

1. Enter `beginundoblock` in the Command Input Area.
2. Perform the sequence of operations that you want to be able to undo.
3. Enter `endundoblock` in the Command Input Area.

**To undo the operations in an Undo block:**

- Choose *Undo action* from the Edit menu, press CTRL+Z, or click the Undo/Redo button in the toolbar.

As for a single action, the Undo option for a block changes to Redo once you have used it.

Maestro can perform certain actions (such as job monitoring) from within undo blocks. These actions might prevent the entire sequence of operations from being undone.

## 2.12 Running Maestro Commands

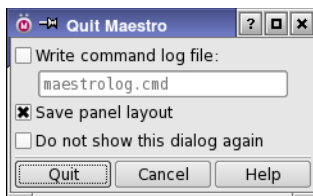
Maestro uses a command language for performing most of its operations. You can use this language in Maestro, by entering commands in the Commands text box, also known as the Command Input Area. To display this tool, choose Window → Command Input Area, or type CTRL+SHIFT+I. The commands are given in the *Maestro Command Reference Manual*.

The Commands text box has access to the command history, which you can navigate with the UP ARROW and DOWN ARROW keys. When you start typing a command, a completion list is shown below the text box, and you can choose the desired command from this list.

## 2.13 Ending a Maestro Session

To end a Maestro session, choose Quit from the Maestro menu, or type CTRL+Q. The Quit Maestro panel opens, offering some choices of actions to be performed when Maestro quits.

To save a log file with a record of all operations performed in the current session, select Write command log file, and enter a name for the log file in the text box. This information can be useful to Schrödinger support staff when responding to any problem you report. This option is also available in the Preferences panel, under General – Quitting Maestro.



**Figure 2.5. The Quit Maestro panel.**

To save the layout of all panels that you have had open in the Maestro session, select **Save panel layout**. The size and position of all the panels is saved for the next Maestro session. This option is also available in the Preferences panel, under **General – Quitting Maestro**.

If you do not want the Quit Maestro panel to open, select **Do not show this dialog again**, or deselect **Warn when quitting Maestro** in the Preferences panel, under **General – Quitting Maestro**. Maestro quits in future with the preferences you have set for quitting.

When you have made your choice, click **Quit**. If you are working in a scratch project and have not saved the project, you are prompted to do so, if you have the preference **Warn before closing a scratch project set**, under **Project – Closing projects** in the Preferences panel. If this preference is not set, the scratch project is discarded.

If you decide that you do not want to end the session, click **Cancel**.

To quit Maestro quickly without setting options, press **CTRL+Q ENTER** (⌘Q ENTER).

# Importing and Exporting Structures and Data

The primary place for reading and writing data from Maestro is a project. When you open a project, the structures and data from that project are read into Maestro. As you modify structures and data they are automatically saved in the project (unless you have set a preference not to do so). Projects are described in detail in [Chapter 9](#). In addition to reading and writing to projects, Maestro can also read and write structural information in a variety of formats, including its own native Maestro format, MacroModel, Jaguar, PDB, MDL SD, Sybyl Mol2, and MCPRO zmat format. Structural information can also be obtained from the input and output files of a wide variety of quantum chemical programs.

Obtaining structures from a file in Maestro is called *importing* rather than *reading* because the structures are imported into the current project. Any structures that do not exist as entries in the current project are external to the project, and therefore must be imported. Similarly, the term *exporting* is used instead of *writing* because a file is created for use outside the current project.

Data that is associated with structures can also be imported and exported independently to spreadsheet files. This capability enables properties that are created by Schrödinger software to be read by a spreadsheet program, manipulated, and re-imported into the project.

## 3.1 Importing Structures

The main means of importing structures is by using the Import panel. You can import data from files in Maestro, MacroModel, PDB, Sybyl Mol2, MDL SD, and a range of other formats. If the files contain multiple structures, such as the output of a conformational search, you can select the structures to import.

When importing structures, Maestro places each structure into a separate, new entry in the current project. For Maestro files, molecular representation information can be imported along with a structure. In addition, Maestro adds two properties to the structures on import: the full path to the file from which the structures were imported (Source Path), and the file name without the path (Source File). If these properties already exist in the imported structures, they are overwritten.

You can undo the import operation, but the changes made to the Project Table remain.

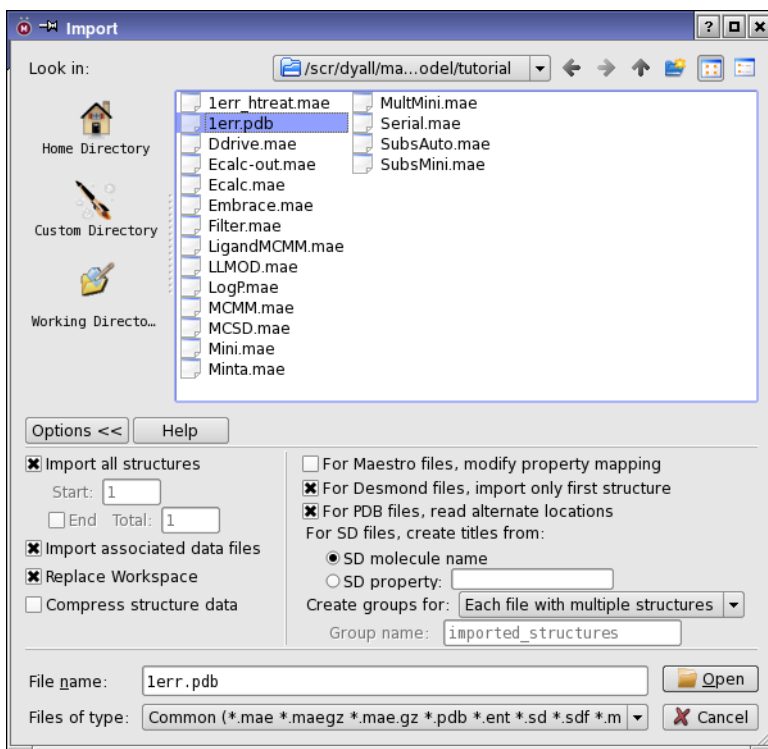


Figure 3.1. The Import panel.

To open the Import panel, do one of the following:

- Choose Project → Import Structures in the main window.
- Press CTRL+I (⌘I) with the pointer in the main window.
- Choose Table → Import → Structures in the Project Table panel.
- Click the Import button on the Project toolbar in the main window or the Project Table panel.



### 3.1.1 Selecting Files

**Selecting a file type:** Before you choose files, you must specify the file type by choosing a file format from the Files of type option menu. The menu options are described below.

#### Common

Import one of the common file types, including Maestro, PDB, and SD. See the descriptions below for these file types.

#### Maestro

Import from Maestro structure files, which have a `.mae` extension (`.mae.gz` or `.maegz` if they are compressed). Properties are imported as well as structures.

#### PDB

Import PDB files, which have either a `.pdb`, a `.pdb.gz` (for compressed files), or a `.ent` extension. (See also [Section 3.1.6 on page 48.](#))

The PDB ID is used for the structure title, and the title from the PDB file is stored in a new property, PDB TITLE.

Where multiple sets of coordinates (alternate positions) exist for atoms in a single PDB entry, Maestro reads all sets by default. You can read the coordinates for the first set only by deselecting Read alternate locations in the Import Options dialog box. Properties are imported as well as structures.

**Note:** PDB structures that have varying number of atoms in different MODELS cannot be imported.

#### Mol2

Import Sybyl Mol2 files, which have a `.mol2` extension.

#### SD

Import MDL SD files, which have an `.sd` or `.sdf` extension for multiple structure files, an `.sdfgz` or `.sdf.gz` extension for compressed multiple structure files, or a `.mol` extension for files with a single structure. Properties are imported as well as structures. If you want to choose a property from the SD file to use for the Title property in the Maestro project, you can do so in the Import Options dialog box. The default is the SD molecule name.

### SMILES

Import SMILES strings from a text file with a `.smi` extension or a compressed text file with a `.smigz` or a `.smi.gz` extension. The text file must have one SMILES string per line, with an optional title separated by a blank. The structures created on import are 2D structures with hydrogens, so you must convert them to 3D structures before using them in applications.

### Jaguar Input

Import from Jaguar input files, which have `.in` extensions.

### ReagentPrep

Import ReagentPrep structure files, which have `.bld` extensions. These are special files labeled with grow bonds for use in CombiGlide.

### MacroModel

Import from MacroModel input or output structure files, which have `.dat` or `.out` extensions. Properties are imported as well as structures.

### Jaguar Output

Import from Jaguar output structure files, which have `.out` extensions. Properties are imported as well as structures.

### MCPRO Input

Import from MCPRO<sup>+</sup> input files, which have `.zmat` extensions.

### Desmond

Import Desmond composite model system files, which have a `.cms` extension if uncompressed, or a `.cms.gz`, or `.cmsgz` extension if compressed.

### Glide Pose Viewer

Import Glide pose viewer files, which are Maestro files that have the receptor as the first entry, followed by a set of docked ligands. These files have a `_pv.mae` extension if uncompressed, and `_pv.mae.gz` or `_pv.maegz` if compressed. There

### Other formats:

Import structures from a range of other programs or formats, including BioGraf, GAMESS output, Gaussian, Mopac, XYZ (MYZ is a synonym for multiple structures in XYZ format), CCF, CIF, mmCIF, and FHI-aims. The format conversion is performed with the use of the program Babel. The list of formats provided here is a subset of the formats that Babel can



convert. If you want to import structures in formats not listed here using Babel, you can use Jaguar to read the files. See [Section 11.1.3](#) of the *Jaguar User Manual* for more information, including the full list of file types read by Babel.

On Linux hosts you can use Babel from the command line to convert structures to a format that Maestro can import directly. To do so, you must first set the environment variable `BABEL_DIR`:

```
csh/tcsh:    setenv BABEL_DIR $SCHRODINGER/mmshare-vversion/data/babel
bash/ksh:   export BABEL_DIR=$SCHRODINGER/mmshare-vversion/data/babel
```

To obtain usage information, enter the `babel` command without arguments:

```
$SCHRODINGER/mmshare-vversion/bin/platform/babel
```

Here, *version* is the 5-digit mmshare version number, and *platform* indicates the platform on which you are running, e.g. `linux-x86`.

Any

Import a file of any type. The file type is determined from the extension of the selected file or the file name you enter in the Selection text box. If the extension is not unique, Maestro does not import the file. The formats for which Maestro recognizes the extension are Maestro, Mol and Mol2, PDB, SD, XYZ (or MYZ), Mopac Cartesian and Internal, and Spartan. This option is useful if you want to locate any of these kinds of structure files.

**Filtering the file list:** To filter the list of files according to your own requirements, choose Custom File Filter from the Files of type option menu. The Custom File Filter dialog box opens, in which you can enter the filter. The filter can include metacharacters for filename expansion: \* for zero or more characters; ? for a single character, and square brackets for specific characters or a range of characters, e.g. `[a-e]`.

**Selecting a directory:** To specify the directory from which to import, you can enter it in the File name text box, or navigate to it using the standard locations, the navigation buttons, or the option menu at the top of the panel. The path displayed in the option menu and the lists are then updated for the chosen directory.

**Selecting a file:** To select a file, you can type its name (and path) in the File name text box, or select it from the list.

If you type the name of the file in the File name text box, you must include the correct extension. In the list of files, only files with the correct extension are displayed.

If the file does not appear in the list, check that you have chosen the correct file type from the Files of type option menu, or select All from this option menu to view all files.

**Selecting multiple files:** You can import structures from more than one file at a time. To select multiple input files, use the SHIFT and CTRL keys in combination with mouse clicks to select as many files as you wish in the Files list, or click All Files to select all files in the Files list.

### 3.1.2 Selecting Import Settings

Once you have selected the files to import structures from, you must choose which structures to import and how to display them. The options for these tasks are hidden by default, and can be displayed by clicking Options. In addition to the options shown in the panel, there are some options that can be set as preferences in the Preferences panel—see [Section 14.2.4 on page 339](#). These options are also described below.

**Selecting structures to import:** Maestro can import multiple structures from multiple files. If you do not want to import all structures from each file, deselect Import all structures. You can then enter the index of the first structure in the Start text box, and the total number of structures to import in the Total text box. You can import to the end of the file by selecting End instead of specifying the total number. These settings are applied to all files: they cannot be set for each file in a multiple file selection. To import different numbers of structures from a set of files, select each file in turn and set the number of structures to import.

If you want to import only the first structure from a Desmond CMS file, select For Desmond files, import only first structure.

**Importing associated data:** If the structure file has other data associated with it, the data can be imported into the project and associated with the relevant entries, by selecting Import associated data files. The mapping of the data to the entries is done in a file with the suffix .smap. This option is selected by default.

**Reading alternate positions from PDB files:** If the PDB file contains alternate positions, you can read them by selecting For PDB files, read alternate locations. If this option is not selected, the coordinates for the atoms with the highest occupancy are read, and the rest are ignored. You can display alternate positions from the Workspace menu.

**Creating titles for SD structures:** SD files often do not have a title property, so you must choose one to display in the project from the options under For SD files, create titles from. The default is SD molecule name. To specify an alternative property for the title, select SD property and enter the property name in the text box.

**Creating groups:** Structures can be added to the Project Table as single entries or as groups. You can control how the entries are grouped on import by selecting an item from the Create groups for option menu. By default, groups are created for files with multiple structures. The groups are named after the file, minus the extension. You can also create a single group for all structures from all imported files, and provide a name in the Group name text box.

**Mapping Maestro and SD properties:** To map properties in an input Maestro file to different properties in the project, select For Maestro files, modify property mapping. This allows resolution of property types as well as creation of a single project property from multiple sources. The Map Properties dialog box opens when you click Open. In this dialog box you can select a property from the project for each property in the input file (in the first structure). You can also save and load property mappings, so you can use different mappings for different files or projects. Mapping of properties in SD files can be done similarly by setting a preference under Project – Importing Structures in the Preferences panel—see [Section 14.2.4 on page 339](#).

At the same time, you can select the properties to import, using the check boxes in the Import column of the Map Properties dialog box. Properties that are not imported cannot be mapped.

**Selecting structures to display:** When you import structures from a file, you can set options to control which structures to display, and whether the structures already in the Workspace are cleared or not. If Replace Workspace is selected (the default setting), Maestro automatically clears existing structures from the Workspace. To import new structures without removing the Workspace contents, deselect Replace Workspace.

Other display options are available under Project – Importing Structures in the Preferences panel—see [Section 14.2.4 on page 339](#). Some of these are described below.

- To specify which structures are to be included in the Workspace, choose one of the options from the Include in Workspace option menu: No Imported Structures, First Imported Structure, or All Imported Structures. The default is First Imported Structure. If you choose No Imported Structures and Replace Workspace is selected, the Workspace is cleared.
- Structures that are imported are not necessarily centered on the coordinate origin, and might not be visible even though displayed. To ensure that the view is centered on the structures and zoomed to display all atoms upon import, select Fit to Workspace following import. (This setting is persistent between Maestro sessions.)

**Opening the Protein Preparation Wizard:** If you are importing a PDB file, you can select Open Protein Preparation Wizard after importing PDB file under Project – Importing Structures in the Preferences panel, to open the Protein Preparation Wizard panel automatically when the structure is imported. You can then prepare the protein for use in various applications.

**Setting up pose viewing:** If a pose viewer file is imported, you can perform the setup in the Project Table automatically by selecting For pose viewer files, turn on pose viewing under Project – Importing Structures in the Preferences panel. You can then immediately start viewing poses—see [Section 6.1](#) of the *Glide User Manual* for more information. This option is selected by default.

### 3.1.3 Interacting with the Import Process

If the import takes more than a few seconds, or there are errors on import, the Import Progress dialog box opens. The dialog box shows which file is being read and how many structures have been read. It also shows whether there have been any errors or warnings on import, and shows the related messages in a text area. You can show or hide these messages by clicking the Details button. You can also copy and paste the messages into another application with the usual key strokes.

You can suspend import by clicking the Pause button. This allows you to examine any messages that were generated, and choose whether to continue with the import or cancel it. The button changes to Resume, so you can continue the import.

If you cancel the import, the structures imported successfully are kept. If you want to delete these structures, click the Undo button or choose Edit → Undo in the main window.

When the import finishes, the dialog box remains open if there were any errors or warnings, or if the messages area is displayed. The Cancel button changes to OK so that you can dismiss the dialog box when you have finished examining the messages.

### 3.1.4 Importing Structures from Another Project

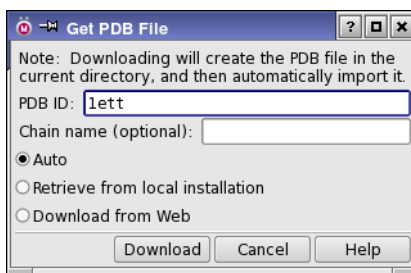
You can import entries from another project, by choosing Project → Import from Project. A project selector opens, in which you can select the desired project. When you have selected the project, the Import entries dialog box opens. This dialog box lists the title and the PDB ID for the entries, which you can select for import. When you click OK, the entries are imported, along with all their properties and auxiliary data. The entries are selected, and the inclusion of entries is governed by the options in the Import panel.

### 3.1.5 Importing Structures by Dragging onto the Workspace

You can import structures into Maestro by dragging one or more files from your window manager's file explorer onto the Maestro Workspace. The structures are imported in the same way as using the Import panel, except that the first structure in the first file is added to the Workspace, and the imported structures are added to the selection in the Project Table. Drag-and-drop is supported for Maestro, SD, MOL2, XYZ, and PDB formats.

### 3.1.6 Importing Structures from the PDB Database

In addition to importing PDB files, you can import structures directly from the PDB database or from a local copy of the PDB database. To do so, you can use the Get PDB File dialog box, which you open from the Project menu. This dialog box runs the `getpdb` utility, which is



**Figure 3.2.** The Get PDB File dialog box.

described in [Section 2.3](#) of the *General Utilities* manual, and which you can use directly from the command line under Unix to extract a structure or a chain into a PDB file.

#### To import a PDB file:

1. Choose Project → Get PDB or click the Get PDB toolbar button.



2. Enter the PDB ID in the PDB ID text box.  
The ID can be in lower case or upper case.
3. If you want to download only a single chain, enter the name in the Chain name text box.
4. Select Auto, Retrieve from local installation or Download from Web.  
Auto tries the local installation first, then downloads from the web as a fallback.
5. Click Download.

The structure is copied to your current directory as a PDB file and imported into Maestro, then the dialog box closes. If you choose to retrieve the file from a local installation, the installation used is the first found in the following list of locations:

- `$SCHRODINGER_PDB`
- `$SCHRODINGER_THIRDPARTY/database/pdb`
- `$SCHRODINGER/thirdparty/database/pdb`

### 3.1.7 Error Reporting for PDB Files

When Maestro imports structures from PDB files, it attempts to place bonds according to a set of standard residue templates, the CONECT records of the PDB file, and geometry. A few amino acids require that choices be made as to where to place the double bonds and formal charges. Schrödinger's conventions for these choices are given in [Table 3.1](#).

If the placement of bonds or identification of atoms fails, the regions of the structure in which problems were identified are assigned an atom property (`i_m_pdb_convert_problem`) that records the type of error. This property can be used to color the structure by the conversion status, with the PDB Conversion Status color scheme. The color scheme is given in [Table 3.2](#). This scheme is not used by default, but you can set a preference to color the structure by conversion status on import in the Preferences panel—see [Section 14.2.4 on page 339](#).

*Table 3.1. Placement of double bonds and formal charges for imported amino acids.*

Amino Acid Pair	Double Bond	Formal Charge
ARN/ARG	between CZ and NH1	for ARG, +1 formal charge on NH1
ASP/ASH	between CG and OD1	for ASP, -1 formal charge on OD2
GLU/GLH	between CD and OE1	for GLU, -1 formal charge on OE2

*Table 3.2. Coloring scheme for structures imported from PDB files.*

Color	Description
orange	Non-standard residues connected by geometry and/or CONECT records. Unless duplicate CONECT records are specified, only single bonds are assigned, so you will need to add multiple bonds.
red	Standard residue, but the input PDB file had missing atoms.
blue	A standard residue that has some atom names unknown to the standard connection template. The unrecognized atom names were connected by geometry.
cyan	An adjacent residue is listed in the SEQRES records but is entirely missing from the ATOM records, indicating a gap in the structure.
green	A residue with alternate positions for the atoms, indicating partial occupancies. By default, all sets of positions are read and stored in the entry. The first set is the set that is displayed by default.
gray	Standard residues connected by standard templates. Confidence in bond orders assigned to these residues is high.

Table 3.3. PDB conversion warning messages.

Status	Message and Explanation
OK	No message. Conversion appears successful.
WARNING	“Problems found while converting file.” A temporary PDB output file was generated successfully, but the assignments were not all successful.
ERROR	“Could not convert file to <i>formatname</i> format.” The conversion failed, usually because the temporary output file could not be created. There may be a permissions problem, or the disk may be full. Another reason for failure is the attempt to convert a file that has varying number of atoms in different MODELS.

Maestro imports PDB files by running the utility `pdbconvert`, which is described in [Section 1.3](#) of the *General Utilities* manual. The conversion creates a temporary Maestro file, and imports the structures from this file. Maestro displays warnings to indicate the status of the PDB conversion, which are listed in [Table 3.3](#). The atom property is stored in the project, and can be used to select residues in the Atom Selection dialog box.

### 3.1.8 Entry Names for Imported Structures

The names of project entries are not required to be unique. Maestro creates entry names that are unique within the file imported by appending the index of the structure in the file to the file base name. Thus, if you import structure 5 from file `mystruct.mae`, the entry name would be `mystruct.5`. If valid entry names already exist, Maestro does not overwrite them.

### 3.1.9 Reading Jaguar Input Files

Jaguar maintains its own input files, which include calculation options in addition to the molecular geometry, and may also include molecular orbitals. Therefore, Jaguar has a separate file reading mechanism. When you read input files through Jaguar, the structures are displayed in the Workspace and Maestro-formatted files are created.

To read input files through Jaguar, choose a task from the Jaguar submenu of the Applications menu, then click `Read` in the Jaguar panel. The Jaguar Read file selector is displayed. Navigate to the directory containing the file, and select the file. Choose the file type from the File Format option menu, and change the Read as setting if necessary. Click `OK` to read the file.

For more information, see the *Jaguar User Manual*.

## 3.2 Exporting Structures

Using the Export dialog box, you can write out structure files in Maestro, PDB, Sybyl Mol2, MDL SD, and SMILES formats, and in various other formats available through the program Babel. You can use the Workspace contents or selected project entries as input, and you can append structures to an existing file and retain additional information when the file format allows it. When exporting project entries, Maestro provides options for exporting each selected entry to its own file, or placing all selected entries in the same file.

Project data is automatically saved, unless you are running in a non-automatic synchronization mode. The structures from a project are saved in a Maestro-formatted file, along with other data. If you want to save just the structures and their associated data, or if you want to save structures in other file formats, you can export the structures.

To open the Export dialog box, do one of the following:

- Click the Export button in the main window or in the Project Table panel.



- Choose Project → Export Structures in the main window.
- Choose Table → Export → Structures in the Project Table panel.
- Choose Export Structures from the entry group shortcut menu.

The Export dialog box is laid out in a similar fashion to the Import dialog box, as a standard file selector, with an Options button to display or hide the options for making export settings. The options are displayed by default.

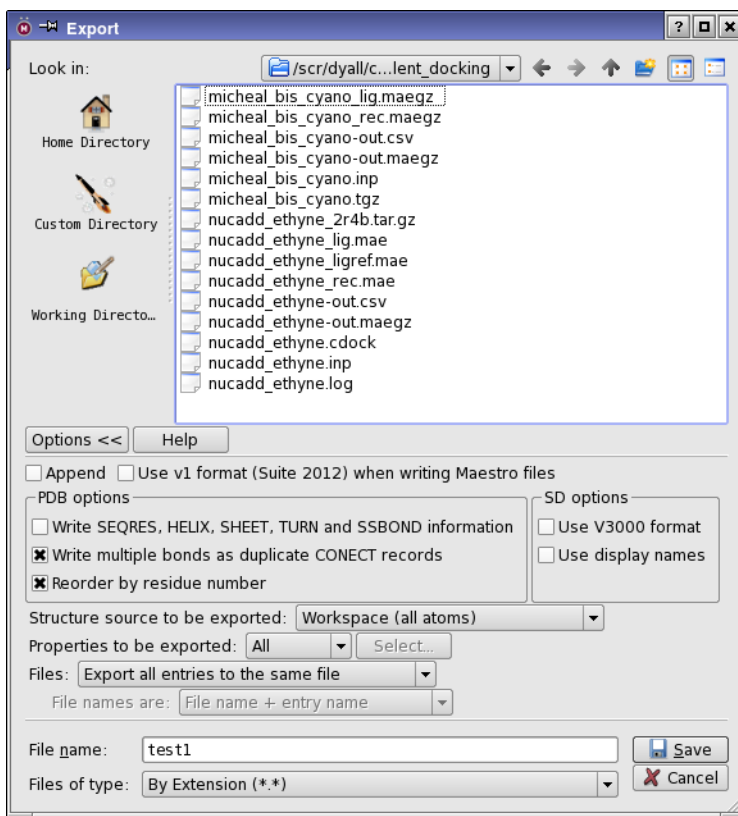
When you have made all the necessary selections, click Export. A dialog box confirms that the files were written. If a file by the specified name already exists, the Exporting-Overwrite? dialog box is displayed and you must choose an action.

### 3.2.1 Selecting a File

By default, structures are exported to a single file, which you can select as described below. It is also possible to export structures to multiple files.

**Selecting a file format:** To create a file, you must specify the file format. By default, the file type is determined by extension, which means that you can enter the file name with its extension in the File name text box. You are warned if the extension is invalid. Otherwise, you can select the type of file you wish to write from the types given in the Files of type option menu, which include Maestro, PDB, Mol2, SD, MacroModel, and a range of file types converted by Babel. The file extension in most cases is determined by the file type. Maestro, PDB, and SD files can be exported as compressed (gzipped) files. Default file extensions for the files in the





**Figure 3.3. The Export dialog box.**

first section of the menu can be set under General → File extensions in the Preferences panel. Properties from the Project Table are exported as well as structures to Maestro and SD files, and any relevant properties are exported to PDB files. SMILES files are exported as plain text files with the extension `.smi`. The SMILES string for each structure is written on a separate line, followed by the title (if it exists), from which it is separated by a space.

**Selecting a directory:** To specify the directory to export to, you can enter it in the File name text box, or navigate to it using the standard locations, the navigation buttons, or the option menu at the top of the panel. The path displayed in the option menu and the lists are then updated for the chosen directory.

**Selecting a file:** If the file exists, you can select it from the list of files or enter its name in the File name text box. If you want to export to a new file, enter the name in the File name text box, including an absolute or relative path if you want.

### 3.2.2 Selecting Export Settings

Once you have selected the file to export structures to, you can make choices about which structures to export and how to export them. You can display the options for these choices by clicking Options.

**Appending or overwriting files:** To append a structure to an existing file, select Append. If the file exists and you do not select Append, it is overwritten.

**Maestro file format:** If you want to export a Maestro file for use in an earlier release, you can select Use v1 format (Suite 2012) when writing Maestro files. The v2 format reduces the size of the Maestro file by removing redundant space and information, so it cannot be used in earlier releases.

**PDB file records:** When writing a PDB file, you can include the SEQRES, HELIX, SHEET, TURN, and SSBOND records in the file by selecting Write SEQRES, HELIX, SHEET, TURN, and SSBOND information. You can write out duplicate CONECT records to store information on the bond order, by selecting Write multiple bonds as duplicate CONECT records. If you deselect this option, only one record is written per bond, regardless of bond order.

You can also ensure that the atoms are written out in ascending order of residue number, by selecting Reorder by residue number. This option ensures that all the atoms from a given residue are in a contiguous block in the PDB file. It is useful if atoms have been added to the structure, as added atoms are placed at the end of the atom list and are not next to other atoms from the same residue.

**SD file format:** If you are saving an SD file, you have the choice of writing it in V3000 format by selecting Use V3000 format when writing SD files. This is a free-format version that allows the writing of structures with more than 999 atoms. The default is to use the V2000 format for SD files, which is fixed-format.

The property names in the SD file can be written out with names as they appear in the Project Table (the *display* name), by selecting Use display names when writing SD files. The default is to write the internal names, which have prefixes that indicate the type and origin of the property and spaces replaced with underscores. When an SD file from another source is imported, the property names do not have type and origin information. The name in the SD file is used as the display name, and an internal name is constructed that adds the type and origin prefixes, for internal use in Maestro. If you are exporting a file for use in other applications, you should select this option, particularly if you are transferring data between Maestro and other applications using SD files and want to maintain consistent naming.

**Specifying the source of the structures:** You can save structures directly from the Workspace or write files containing structures from one or more project entries. To write out the contents of the Workspace to a file, choose Workspace (all atoms) from the Structure source to be exported option menu. This is equivalent to writing the included entries. If you only want the displayed atoms to be written to a file, choose Workspace (Displayed atoms only). The atoms are written as a single structure, even if there are multiple entries in the Workspace. To write out the entries that are selected in the Project Table, choose Project Table (selected entries). If there are no selected entries in the Project Table, Workspace is selected by default.

**Specifying the properties to export:** You can export all properties from the Project Table, the properties that are shown in the Project Table, or the properties that you select, by choosing All, Shown, or Selected from the Properties to be exported option menu. To change the shown properties, choose Property → Show in the Project Table panel. To select properties for export, choose Select from the option menu, then click the Select button. A property selector opens, in which you can choose the properties. The property selection is stored in the project for later use and as a user preference. Initially, the selection is set to the shown properties.

The properties are written in the order in which they appear in the Project Table. You can change the order of the properties in the Reorder Properties dialog box (see [Section 9.11.14 on page 244](#)).

**Exporting to single or multiple files:** You can export entries to a single, multi-structure file, to multiple files each of which contains a single entry, or to multiple files each of which contains all the entries from a single entry group. From the Files option menu, choose Export all entries to the same file, Export each entry to a different file, or Export each entry group to a different file. If you export to one of the Babel-supported formats, you can only export a single structure to each file, so you must choose Export all entries to a different file. The exception is XYZ (or MYZ) format, which supports multiple structures in a single file.

### 3.2.3 Exporting Multiple Files

If you want to save each entry or each entry group to a separate file, you must specify how to name the files by choosing one of the naming schemes from the File Names Are option menu. The naming schemes are described below.

**Note:** Because entry names, entry titles, and group titles are not unique, choosing any option that involves the names or titles does not guarantee that the file name is unique. You must make sure that these names or titles are unique. Otherwise, Maestro will offer to either overwrite a previously created file with the same name or to skip writing the file, and in either case not all the entries will be exported.

File name + entry name

File name + group title

If you choose File name + entry name or File name + group title, you must select a file or type in a file stem. The entry name or group title and the file suffix are appended to the file stem. If you choose a file name, the suffix is the suffix of that file name. For example, if you are exporting the entries combination-3, combination-4, and combination-5 as separate files, and you select the file `structure.maegz`, the new files are named

```
structure_combination-3.maegz
```

```
structure_combination-4.maegz
```

```
structure_combination-5.maegz
```

If you typed in the file stem `HIV`, the following files would be written, with the default extension `.mae` (or the extension for the selected file type):

```
HIV_combination-3.mae
```

```
HIV_combination-4.mae
```

```
HIV_combination-5.mae
```

File name + entry ID

File name + group ID

If you choose File name + entry ID or File name + group ID, you must select a file or type in a file stem. The entry ID or group ID and the file suffix are appended to the file stem. If you choose a file name, the suffix is the suffix of that file name. For example, if you are exporting the entries with IDs 3, 4, and 5 to separate files, and you select the file `structure.mae`, the new files are named

```
structure3.mae
```

```
structure4.mae
```

```
structure5.mae
```

File name + automatic number

If you select File name + automatic number, you must specify a filename. The files are given the same name and extension as the selected file, but numbers are added in sequence to the base file name. For the example above, with the file `structure.mae`, the new files are named

```
structure_1.mae
```

```
structure_2.mae
```

```
structure_3.mae
```

#### Just entry names

If you choose Just entry names, the file name is constructed from the entry name, and the File name option menu becomes unavailable. You can choose the file type from the Files of type option menu as usual. For the above example, the new files are named

```
combination-3.mae  
combination-4.mae  
combination-5.mae
```

and a dialog box confirms that the files were written to the desired directory.

#### Just entry titles

#### Just group titles

If you choose Just entry titles or Just group titles, the file name is constructed from the entry title or group title, with special characters and blanks replaced with underscores (`_`). For two entries with titles “Acetic acid” and “Methyl salicylate”, the new files are named

```
Acetic_acid.mae  
Methyl_salicylate.mae
```

The File name option menu is unavailable in this case. You can choose the file type from the Files of type option menu as usual.

### 3.3 Exporting Data to a Spreadsheet

The Project Table does not have full spreadsheet capabilities, but you can export data to a spreadsheet file, manipulate it in a spreadsheet program, then re-import it into Maestro. Exporting data to a spreadsheet file is done from the Export Spreadsheet panel. The data that you can export are the properties in the Project Table. To export data, you must first open Project Table panel, which you can do by choosing Project → Show Table in the main window or clicking the Open/Close project table button on the toolbar.

When the Project Table panel is displayed, choose Table → Export → Spreadsheet. The Export Spreadsheet panel is displayed. The layout of this panel is similar to that of the Export and Import panels, with standard file navigation and selection tools, and an Options button for showing and hiding the settings.

**Selecting a directory:** To specify the directory to export to, you can enter it in the File name text box, or navigate to it using the standard locations, the navigation buttons, or the option menu at the top of the panel. The path displayed in the option menu and the lists are then updated for the chosen directory.

**Selecting a file:** If the file exists, you can select it from the list or enter its name in the File name text box. If you want to export to a new file, enter the name in the File name text box. You can specify an absolute or relative path in the File name text box in addition to the file name. Existing files will be overwritten.

The selection of entries, properties and delimiter is made in the settings section, which you show or hide by clicking Options.

**Selecting entries to export data from:** The Entries option menu allows you to choose different classes of entries to export data from: All, Shown, Selected, and Included. The default is All. For more information on showing, selecting, and including entries, see [Section 9.5 on page 197](#) and [Section 9.6 on page 203](#).

**Selecting properties to export:** You can choose whether to export all properties, the shown properties, or your choice of properties by selecting All, Shown, or Selected from the Properties option menu. The row number and the inclusion state are not exported. All other properties can be exported, including the Booleans represented in the Title column for the auxiliary data. To limit the range of properties exported, you can hide columns by using the Properties shortcut menu in the Project Table panel (right-click in the column heading), then export only the shown properties. Alternatively, you can choose the properties to export, by choosing Selected from the Properties option menu, clicking Select, and selecting the properties in the property selector that opens. The property selection is stored in the project for later use and as a user preference. Initially, the selection is set to the shown properties.

The entry title is always in the first column in the exported file.

**Selecting a delimiter:** You can choose from the two standard delimiters, a comma and a tab character, or choose other, then enter your own delimiter in the text box.

Once you have made your selection, click Save in the Export Spreadsheet panel.

### 3.4 Importing Data From a Spreadsheet

Once you have exported data from Maestro and manipulated it in a spreadsheet, you can re-import the data into Maestro. You can also import data that did not originate from Maestro. Importing data from a spreadsheet file is done from the Import Spreadsheet dialog box, and the data is added to entries in the Project Table. The data that you import must therefore match entries in the project. For data that you exported from Maestro, matching should be no problem, but for data that did not originate from Maestro, you must ensure that there is a proper match to the entries in the Project Table.

To import data, you must first open the Project Table panel, which you can do by choosing Show Table from the Project menu in the main window, or clicking the Open/Close project table button in the toolbar.



When the Project Table panel is displayed, choose Table → Import → Spreadsheet. The Import Spreadsheet panel is displayed. Like the Export and Import panels, this panel is a standard file selector, with options added. To select a file to import data from, you can navigate to it with the file selection tools, or enter its name in the File name text box.

When the properties are imported, you can add them to the selected entries or to all entries, by selecting an Import properties for option.

If you want to add values only where the project does not have values, deselect Overwrite existing data. Otherwise, existing values are replaced with values from the spreadsheet and new values are added.

When you have selected the file and set any options, click Open. The Choose Import Key dialog box opens. In this dialog box, you determine how the rows of the spreadsheet are mapped to the entries in the Project Table, and select the delimiter. The File key column lists the properties in the spreadsheet file. The values of the key that you choose in this column are matched to the values of the property that you choose in the Match to property in Project Table column. You must choose a property from each column—for example, if both the spreadsheet and the Project Table have a Title property, you can match the rows by title. If the file key value for a given row in the spreadsheet matches more than one entry, the properties for that row are copied to all entries; if several file key values match a single entry, the row for the last file key value that matches is used to import data.

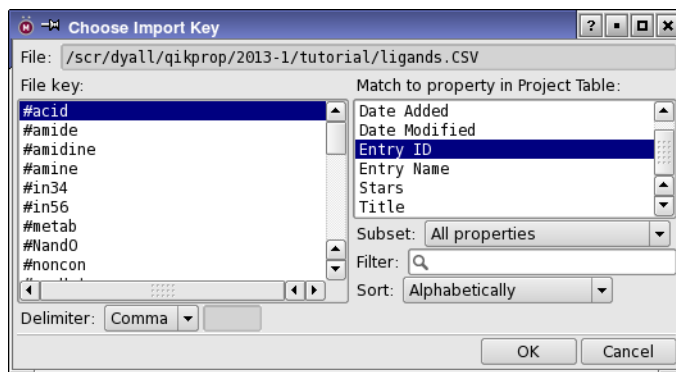
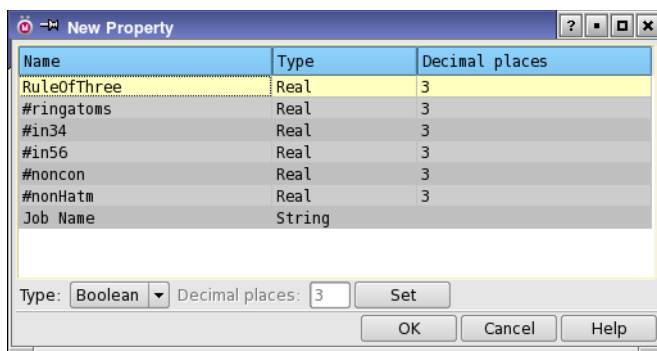


Figure 3.4. The Choose Import Key dialog box.



**Figure 3.5.** The New Property dialog box.

By default, the Entry ID property is selected in the Match to property in Project Table column and also in the File key column if the file contains the entry ID as a property. These defaults allow you to easily import data for entries whose properties were exported: the imported data is associated with the correct entries because the entry ID is unique.

To continue, choose the delimiter that is used in the spreadsheet file, then click OK. If all the properties in the spreadsheet already exist in the Project Table, they are imported immediately.

If any properties do not exist in the Project Table, the New Property dialog box opens. This dialog box lists the property name, the property type (Boolean, Integer, Real, or String), and number of decimal places for real properties. To change the property type, select the properties in the table (use shift-click and control-click for multiple properties), choose the property type from the Type option menu, and click Set. For real properties, you can set the number of decimal places to display in the Decimal places text box before clicking Set. The default precision is set as a preference—see [Section 14.3.1 on page 341](#) for more information. When you click OK, the properties are imported with the specified types.

### 3.5 Exporting Structures and Data to a Canvas Project

You can export the selected entries in the Project Table panel with their properties directly to a Canvas project, and open the Canvas GUI with that project loaded. To do so, choose Table → Export → To Canvas in the Project table panel, or right-click in the selected entries and choose Export to Canvas. The Export to Canvas dialog box opens, and offers the following choices for how the structures are exported:

- New Canvas project—Create a new Canvas project with these structures and properties.
- Existing Canvas projects—Add the structures to an existing project, either by appending the structures, or replacing existing structures.



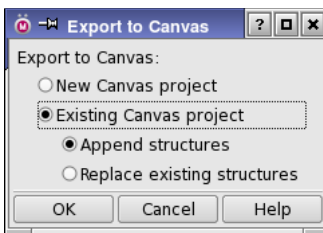


Figure 3.6. The Export to Canvas dialog box.

When you click OK in this dialog box, a file selector opens so that you can navigate to a location and name the new Canvas project or choose the existing Canvas project. Once the project is created or updated, the Canvas GUI is started with the specified project already loaded.

## 3.6 Exporting Data from a Table

You can export data from any table in Maestro, either in CSV or HTML format. To do so, right-click in the table and choose the format from the Export Table Data submenu. A file selector opens in which you can navigate to a directory and enter the file name. The table must have some data in it to export. The file that is written includes the column headings as well as the data. The HTML file contains just the table.

## 3.7 Copying and Pasting Structures

You can import structures by pasting them into the Workspace. The structure must be a SMILES string that was previously copied to the clipboard (*not* the paste buffer on Linux). On Windows, you can copy a structure in ChemDraw or ISIS/Draw and paste it into the Workspace.

A new project entry is created for the structure, with the SMILES string as the title. The structure retains any stereo (R/S or E/Z) properties it has. You can paste the structure in 2D, by choosing Edit → Paste or pressing CTRL+V. SMILES strings are converted to 2D structures, which are then placed with the centroid at the coordinate origin. If the coordinate origin is outside the viewing area, you will not see the structure when you paste it and you will have to click Fit to Workspace to see the structure.

If you want to paste the structure at another location, choose Edit → Paste Special → By Placing, or press CTRL+SHIFT+V, then click in the Workspace where you want the centroid of the structure to be located. The cursor changes to a plain arrow for this operation, because you are picking a point rather than atoms.

If you want to use the structure for modeling, you must convert it to a 3D structure, by using LigPrep for example. The structure retains stereo (R/S or E/Z) properties, which can be used by LigPrep to ensure the correct stereochemistry. A minimized 3D structure can be generated when you paste the structure, by choosing Edit → Paste Special → As 3D. This feature uses tools from LigPrep but does not allow any of the flexibility that is available in LigPrep.

You can also copy atoms from a structure in Maestro with Edit → Copy or CTRL+C (⌘C), and paste them into the Workspace with Edit → Paste or Edit → Paste Special → By Placing. If there is nothing in the Workspace, a new entry is created with a default title. If there is a single entry in the Workspace when you paste, it is added to this entry. If there are multiple entries in the Workspace when you paste, you are prompted to choose an entry to add the atoms to, or to create a new entry. When you copy (or cut) the atoms, any bonds between the copied atoms and the rest of the Workspace structure are broken and capped with hydrogen atoms. You can also paste the copied structure into ChemDraw.

Another option is to copy atoms as a SMARTS pattern, by selecting atoms in the Workspace and choosing Edit → Copy as SMARTS. The SMARTS pattern can then be pasted anywhere that accepts SMARTS as input—into text boxes in other panels in Maestro, for example. You can set preferences for some of the notational elements in the SMARTS pattern—see [Section 14.14 on page 375](#).

# Viewing the Workspace

The view of the objects in the Workspace can be changed in a variety of ways, and you can save the view for later use. This chapter describes the different views that are available, how you can change them, and how you can manage them. It also describes viewing effects such as tiling, stereo viewing, perspective, and fog.

## 4.1 The View Toolbar

The View toolbar provides tools for changing the view of the Workspace. These buttons are described briefly below, and in more detail in later sections. See [Section 2.4 on page 18](#) for general information on toolbars.



**Fit**

Fit the selected atoms (or all atoms, if there is no selection) to the Workspace.

Menu equivalent: View → Fit to Workspace → Selected atoms.



**Fog**

Turn fogging on or off, or select automatic fogging when the Workspace has more than 40 atoms.

Menu equivalent: View → Fog → On/Off/Automatic.



**Enhance**

Enhance depth cues.

Menu equivalent: View → Fog → Enhance Depth Cues.



**Rotate X**

Rotate the Workspace around the  $x$  axis by 90 degrees.

Menu equivalent: View → Rotate X 90.



**Rotate Y**

Rotate the Workspace around the  $y$  axis by 90 degrees.

Menu equivalent: View → Rotate Y 90.



**Tile**

Arrange the Workspace entries in a rectangular grid of “tiles”. From the button menu you can choose to move tiles, transform tiles separately or together, choose how to tile the entries.

Menu equivalent: View → Tile.



**Reset**

Reset the rotation, translation, and zoom of the Workspace to the default state (coordinate  $x$  and  $y$  axes in the plane of the screen,  $z$  axis perpendicular to the screen).

Menu equivalent: View → Reset.

## 4.2 Changing the View

The view that is presented in the Workspace can be regarded as the image that you see through a video camera. Changing the view is like moving the camera to a new location or a new angle, or zooming in or out. Changing the view does not change the coordinates of any of the objects in the Workspace, it merely changes the camera angle, location, and zoom. However, you can apply the current view to change the coordinates of the Workspace objects by choosing **Edit** → **Update Coordinates**.

The view is stored as a coordinate system, with an origin (location), an orientation (angle), and a scale factor (zoom). The coordinate system in Maestro is oriented so that the positive  $z$  axis points out of the screen, the  $x$  axis is the horizontal axis, and the  $y$  axis is the vertical axis. The default view is the coordinate system and scaling of the structures in the Workspace.

Changing the view is done with a “global transformation” of the coordinate system: a translation, a rotation, or a zoom. Rotation, translation, and zoom actions are assigned to combinations of mouse buttons with the **SHIFT** and **CTRL** keys. The default assignments for a 3-button mouse with a scroll wheel are given in [Table 4.1](#). For information on the mappings for this and other mouse or trackpad configurations, open the **Customize Mouse Actions** panel (Maestro → **Customize** → **Mouse Actions**). You should take care that you do not click instead of drag, because clicking might have a particular action associated with it in the context in which you are working, and change the structure. The following sections give more details on doing global transformations.

*Table 4.1. Mapping of Workspace operations to mouse actions.*

<b>Operation</b>	<b>Action</b>
Rotate about the $x$ - and $y$ -axes	Drag with middle mouse button
Rotate about the $x$ -axis only	Drag vertically with <b>SHIFT</b> and middle mouse button
Rotate about the $y$ -axis only	Drag horizontally with <b>SHIFT</b> and middle mouse button
Rotate about the $z$ -axis	Drag horizontally with <b>CTRL</b> and middle mouse button
Spot-center on an atom	Right-click
Translate in the $x$ - $y$ plane	Drag with right mouse button
Translate along the $y$ -axis	Drag vertically with <b>SHIFT</b> and right mouse button
Translate along the $x$ -axis	Drag horizontally with <b>SHIFT</b> and right mouse button
Translate about the $z$ -axis	Drag horizontally with <b>CTRL</b> and right mouse button
Zoom	Drag horizontally with middle and right mouse buttons or with <b>SHIFT+CTRL</b> and middle mouse button; use the scroll wheel; use the pinch gesture.

### 4.2.1 Translating the View

Translations can be carried out with the right mouse button, as described in [Table 4.1](#).

You can perform translations in increments along the  $x$ ,  $y$ , and  $z$  axes with the keyboard keys and the corresponding items under **View** → **Translate**. The keys are described in [Table 2.8 on page 33](#).

You can also do a translation by “spot-centering”, an action that places the coordinate origin of the view on a particular atom, which then appears at the center of the Workspace. As a consequence, subsequent rotations of the view are performed about this atom. This action is done by right-clicking on the atom.

In addition to the mouse controls, a number of global transformations are available from the **View** menu and the main toolbar.

### 4.2.2 Rotating the View

In addition to the rotations that can be performed with the middle mouse button, there are a number of other actions that perform a rotation.

On the toolbar, there are two buttons for rotation by  $90^\circ$  about the  $x$  axis or the  $y$  axis:



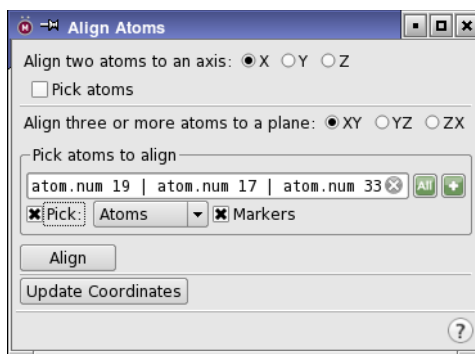
These buttons have corresponding menu items, **View** → **Rotate** → **X 90** and **View** → **Rotate** → **Y 90**.

You can perform rotations in increments about the  $x$ ,  $y$ , and  $z$  axes with the keyboard keys and the corresponding items under **View** → **Rotate**. The keys are described in [Table 2.8 on page 33](#).

Another rotation that you can perform is to align the view so that selected atoms are lying on one of the Cartesian axes or planes. This action is performed in the **Align Atoms** panel, which you open by choosing **View** → **Align**.

To align two atoms to one of the Cartesian axes, select the axis, select **Pick atoms**, then pick the two atoms. A purple cube is drawn around the first atom when you pick it, and the alignment is performed when you pick the second atom. The view is rotated through the smallest possible angle to perform the alignment.

To align three atoms to one of the Cartesian planes, select the plane, then use the picking tools in the **Pick atoms** to align section to pick the three atoms. When the third atom is picked and a check is performed to ensure that the plane is uniquely defined (i.e. the atoms are not collinear), a blue-green plane is displayed in the Workspace, and the **Align** button becomes



**Figure 4.1. The Align Atoms panel.**

available. Click this button to perform the alignment. The view is rotated through the minimum angle required to bring the selected atoms into alignment with the chosen plane. If you do not want to see the plane, deselect Markers.

When you have done the alignment, you can also change the coordinates of the structure to those of the current view, by clicking Update Coordinates. The structure itself is then aligned on the axis or plane, and not just the view of the structure.

### 4.2.3 Zooming In and Out

Zooming in and out can be done with the scroll wheel, with the middle and right mouse buttons (held down together), with SHIFT+CTRL and the middle mouse button, or with the pinch gesture on a trackpad. The keys K and J are assigned to zooming in and zooming out, in small increments. Each press of one of these keys corresponds to one click of the scroll wheel, and you can hold the keys down for continuous zoom.

Another way of zooming is to use the Fit to Workspace button on the toolbar, which zooms in or out so that the atom selection fills the Workspace (or all atoms, if there is no selection).



You can perform a fit to the Workspace from the View menu. The Fit to Workspace submenu offers the choices of Selected Atoms (shortcut Z), All, or Ligand (shortcut L). Choosing All allows you to fit the entire structure to the Workspace without changing the selection.

### 4.2.4 Restoring the Default View

To restore the view to the default view, in which the view axes are aligned with the coordinate axes of the structure, click the Reset View button on the toolbar.



### 4.2.5 Setting the View Origin and Rotation Center

By default, the origin of the view coordinate system moves when you translate a structure, so that rotation of the view has the same effect on the structures no matter where they are translated to. The origin is changed by spot-centering, which was described in [Section 4.2.1 on page 65](#). The origin is reset when you restore the default view, and it is also set when you do a Fit to Workspace.

If you want the center for rotation to stay at the same location regardless of how you translate the structures, you can set a preference in the Preferences panel. Choose Maestro → Preferences to open the panel, then in the Workspace tab, select Keep center of rotation fixed while translating. The rotation center is then decoupled from the translation origin, and remains at the location of the view origin when you selected the option. If you want the center for rotation to stay at the center of the Workspace, reset the view first, then select the option.

If you want to display the center for rotation, select Display center of rotation in the Workspace tab of the Preferences panel.

## 4.3 Saving, Restoring, and Managing Views

When you have set up the view of the Workspace for a particular purpose—for example, with a particular view of a binding pocket—you can save the view for future use. Views can be saved with a name, restored, and even played through. The tools for working with views are available from the View menu and the Saved Views toolbar, which you display by choosing Window → Toolbars → Saved Views, or by clicking the Saved Views button on the Manager toolbar. The toolbar buttons are described below.



#### Save

Save the current view of the Workspace (orientation, location, and zoom) as a saved view. Opens a dialog box in which you can name the view.  
Menu equivalent: View → Save.



#### Previous

Apply the previous view in the list of saved views to the Workspace.  
Menu equivalent: View → Restore View → Previous.



### Next

Apply the next view in the list of saved views to the Workspace.  
Menu equivalent: **View** → **Restore View** → **Next**.

1

### View 1

Apply the first saved view to the Workspace. The other four numbered buttons apply the specified view number. These buttons are always assigned to the first five views listed in the **Manage Views** panel. Buttons that do not have a corresponding view are not available.  
Menu equivalent: **View** → **Restore View** → **ViewN**.



### Manage

Manage the saved views. Opens the **Manage Views** panel, in which you can select views to show, play through views, record movies of the views, import and export views, save and delete views, and animate view changes.  
Menu equivalent: **View** → **Manage Views**.

The **Manage Views** panel contains tools for all view operations. You can open this panel by choosing **View** → **Manage Views**, or clicking the **Manage views** button on the **Views** toolbar.

To save a named view, choose **View** → **Save View** or click the **Save view** button on the **Views** toolbar:



The **Save View** dialog box opens, in which you can enter a name for the view. The default name is *viewN*. If you want to save views with the default name rather than explicitly naming them, you can select **Use default name** under **When saving views** in the **Manage Views** panel. The **Save View** dialog box is no longer displayed, unless you select **Prompt for name**.

The translation, rotation, and zoom are stored in the named view, and the new view is saved in the project. Once the view is saved, it is listed on the **Restore View** submenu of the **View** menu and entered into the table in the **Manage Views** panel. If it is in the top five views in this table, it is associated with a button on the **Views** toolbar.

Named views store information only about the state of the “camera”—the location, angle, and zoom. They do not store any information about the content of the **Workspace**. This means that you can, for example, set up a view of a protein, then at some later point, display the protein from the same angle with a ligand in the binding pocket.

To restore a saved view, use one of the following methods:

- Choose **View** → **Restore View** → *view-name*
- Click the button for the view on the **View** toolbar (if it has one)
- Select the view in the **Manage Views** panel and click **Restore**



In addition to restoring a single view, you can step through a sequence of views manually, or play through a sequence of views with a given display time for each view, and you can export a movie of the sequence of views.

The views that are played can be selected by checking the check box in the Play column of the Views table. Only the checked views are played with the play controls. These controls also apply to saving a movie of the views.

To step through views manually, click the Previous view or Next view button on the Saved Views toolbar, or in the Manage Views panel. You can also use the View → Restore View submenu items to step to the previous or next view.



To play through the views continuously, use the controls in the Manage Views panel.

If you want the view changes to be smooth rather than instantaneous, select View animation in the Animation section, and set the duration of the animation. If the distances the structures move are large, you can control when the animation is used by selecting Limit animation distance and entering the distance above which animation is turned off in the Maximum distance text box.

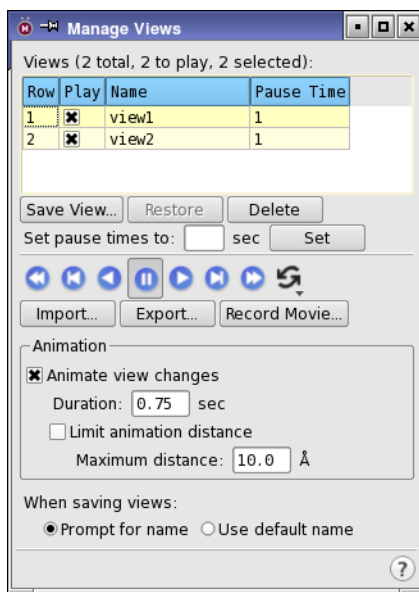


Figure 4.2. The Manage Views panel.

The animation time can be coordinated with the length of time each view is displayed to produce a continuous movement. The view time is set in the **Pause Time** column of the **Views** table. If you want to set the pause time for multiple views, select them in the table, enter a value in the **Set pause times** text box, and click **Set**.

To save a movie in MPEG format with the chosen play list and duration settings, click **Record Movie**, and navigate to a location and name the movie file. The movie does not record animation of view changes.

To delete views, select them in the **Views** table and click **Delete**.

Since views are saved in the project, they are not automatically available when you close the project. To transfer views between projects, you can import and export them, by using the **Import** and **Export** buttons. These buttons open file selectors, in which you can navigate to a location and name the view file.

### 4.4 Tiling the Workspace

Sometimes you want to see several structures or surfaces in the **Workspace** separated from each other, rather than superimposed. This can be done by *tiling* the **Workspace** contents, which rearranges the objects in a grid pattern in the **Workspace**. There are three ways that you can tile the **Workspace**, or tiling modes, which can be selected from the **Tile** submenu of the **View** menu or the **Tile** button menu on the **View** toolbar.

- **Tile by Entry**—This is the default mode, in which each entry in the **Workspace** occupies a separate tile, except for fixed entries, which are displayed in every tile.
- **Tile by Entry Groups**—In this mode, all entries that are in the same entry group are displayed in the same tile. This mode allows you, for example, to display several proteins with their ligands in the **Workspace**, and use the **ePlayer** to step through ligands for a given receptor.
- **Tile by Surface**—In this mode, each surface that is displayed in the **Workspace** is placed in a separate tile, along with the corresponding structure. Surfaces for fixed entries are displayed in every tile, and entries that are displayed in the **Workspace** that do not have surfaces are displayed in their own tiles, at the end of the grid (i.e. they are treated as having a single surface that is null). This mode allows you to display multiple surfaces for a single entry in separate tiles, such as molecular orbitals or **SiteMap** surfaces.

To perform the tiling, choose **View** → **Tile** → **Tile Workspace**, or click the **Tile** button on the **View** toolbar.



The button is highlighted, to indicate that you are in tile mode. To undo the tiling, click the Tile Entries button again. You can also enter and exit tile mode by choosing View → Tile → Tile Workspace or pressing CTRL+L. Information on individual transformations is discarded when you exit tile mode.

The tiles are initially arranged according to the order in which the entries were included in the Workspace. There are two ways of rearranging the tiles. The first is to exclude an entry and then include it again. This entry is placed at the end of the grid of tiles. The second is to move individual tiles. To move tiles, first choose Pick Tiles to Move from the Tile button menu or from the Tile submenu of the View menu. Then click on a tile to select it for moving, and click on the desired new location. The tiles between the initial location and the final location are moved to fill the space left by moving the selected tile, and the selected tile is placed in the new location. When you have finished moving tiles, deselect Pick Tiles to Move.

Each tile is a mini-Workspace, in which you can perform all the operations that are available when the Workspace is not tiled. Transformations (rotation, translation, zoom) can be performed on all tiles simultaneously, or on individual tiles. To perform simultaneous transformations, select Transform All Tiles from the Tile entries button menu (or the Tile submenu of the View menu). This option is selected by default. If you deselect this option, you can transform individual tiles. Clicking in a tile selects the tile, which is marked by a thicker border. To transform an individual tile, start the transformation operation when the pointer is in the tile. You can drag outside the tile to finish the transformation operation, but to start another operation on the same tile, you must move the pointer back into the tile.

To reset the view in each tile to the initial view, choose Reset All Tiles from the Tile button menu (or View → Tile → Reset All Tiles). To reset the view in an individual tile, right-click in the tile and choose Reset Tile from the shortcut menu.

To apply the view or zoom for an individual tile to all tiles, right-click in the tile and choose Apply View to All Tiles or Apply Zoom to All Tiles from the shortcut menu.

When the Workspace is tiled, you can save an image that shows the tiled Workspace.

Some actions do not behave the same in tile mode as out of tile mode.

- Adding atoms in Draw or Place mode by clicking in an empty part of the Workspace adds the atoms to the scratch entry. If the scratch entry is not in the tile you clicked in, the atoms will not appear in that tile, but rather in the scratch entry tile. If you draw or place atoms by clicking first on an existing atom, the behavior is normal: atoms are added to the structure that you clicked on.
- Saving a view only saves the current global transformation, and does not preserve changes made in individual tiles. Consequently, restoring a view applies the same view to each tile, and does not preserve changes made in individual tiles.

## 4.5 Using the Full Screen

If you want to make use of the full size of your monitor to view the Workspace, you can enter full-screen mode, by choosing *Workspace* → *Full Screen*, or pressing **CTRL+=**. In this mode, the only components of the main window that are visible by default are the Workspace, the menu bar, and the Auto-Help bar. You can use the *Window* menu to display the toolbars, open hidden panels, and perform other window-related actions.

To exit full-screen mode, press **ESC**.

Another way to make use of your monitor is to simply maximize the main window instead of entering full screen mode. The main window components that you have displayed occupy some space, but you can undisplay many of these components if you want the extra space.

## 4.6 Clipping

How much you can see of the structures that are in the Workspace depends on whether you have zoomed in or out, and also on where the structure is “clipped”. Clipping is used to limit the parts of a structure that are displayed in the Workspace, by defining clipping planes perpendicular to the  $z$  axis (or parallel to the screen) and displaying only the parts of the graphical image that are between these planes. Anything that is in front of or behind these planes is not displayed. Clipping is useful when working with large structures containing many atoms, in which it can be hard to see certain atoms and even harder to pick those atoms.

The part of the structure that is displayed in the Workspace is indicated in the *clipping planes window*. This window is located in the lower-right corner of the Workspace. By default, it is not displayed. You can display it by choosing *Window* → *Clipping Planes*.

The display in the clipping planes window consists of the following features:

- **Top view of structures:** A representation of the structures in the Workspace, drawn in the wire frame representation. The view of the structures is from the top, that is, from the positive  $y$  direction looking down to the negative  $y$  direction. The back of the structure is in the upper part of this window while the front is in the lower part of this window.

Zooming in and out on the structures in the top view is controlled by a preference. If you select *Zoom clipping planes* with *Workspace* under *Workspace* → *Clipping Planes* in the Preferences panel (see [Section 14.4.8 on page 347](#)), the top view zooms in and out as you zoom in and out in the Workspace. If you deselect this option, the top view stays the same, regardless of what happens in the Workspace. Translation in  $x$  and  $z$  moves the displayed structures.

- **Clipping planes:** These are horizontal lines that mark the planes where the graphical image is clipped. The lower line marks the plane that is closest to the viewer, and the upper line marks the plane furthest from the viewer.

The planes can be moved by dragging the horizontal lines. To move both planes in the same direction, hold down the CTRL key and drag one of the planes or use the scroll wheel. To move both planes in opposite directions, hold down the SHIFT key and drag one of the planes or use the scroll wheel. You can use the keyboard to move the planes closer together (F), further apart (G), towards you (=), or away from you (-), in small increments. These actions are also available from View → Move Clipping Planes.

The clipping planes are adjusted if you select Adjust clipping planes when focusing on a substructure under Workspace → Clipping Planes in the Preferences panel (see Section 14.4.8 on page 347) and you do one of the following:

- Select part of a structure and perform a fit-to-Workspace.
  - Perform a fit-to-ligand.
  - Middle-click a residue in the sequence viewer to zoom in on it.
  - Select a residue in the residues table of the Density Fit panel (PrimeX)
  - Select a rotamer in the Residues table of the Rotamers dialog box.
  - Find a residue with the Find toolbar.
- **Viewing volume indicator:** This is a green box that represents the viewing volume. As you zoom in on the structure, the box shrinks. If you have perspective enabled, the viewing volume box is trapezoidal, with the small side at the bottom.

Clipping can be applied to fit objects in the Workspace, by choosing To All Atoms, To Selected Atoms, or To Ligand from the Move Clipping Planes submenu of the View menu. This feature can be used to reset the clipping without changing the zoom.

Clipping can be applied selectively, as well as to all graphical objects. To choose what clipping is applied to, right-click in the clipping planes window and make your choice from the shortcut menu that is displayed. The choices are:

- **All**—Apply clipping to all objects (structures and surfaces). Clipping planes are drawn as horizontal orange lines, and can be adjusted by dragging.
- **Surfaces**—Apply clipping to surfaces but not to structures. There are four clipping planes: front, back, left, and right. These planes are drawn as horizontal and vertical purple lines, and can be adjusted by dragging.
- **Surfaces to selected atoms**—Apply clipping to the surfaces using a cube centered on the selected atoms. For example, you might select just the ligand in a ligand-receptor complex, and the surface will be clipped to a cube that contains the ligand. The outline of the cube is displayed in cyan. You can resize the cube by dragging horizontally.

- Selected atoms—Apply clipping only to the selected atoms. For example, you could select the receptor in a complex, and leave the ligand unclipped. Clipping planes are drawn as horizontal cyan lines, and can be adjusted by dragging.

## 4.7 3D Viewing

Maestro provides several tools to enhance the 3D appearance of complex structures. These tools include stereo viewing, perspective, fogging distant atoms, and depth cues. They are described in the sections that follow. Most of the tools are in the 3D and Fog tabs of the Appearance panel, which you can open by choosing View → 3D Options or View → Fog → Settings.

### 4.7.1 Stereo Viewing

Maestro provides two kinds of stereo viewing method: software stereo and hardware stereo. Software stereo can be run on any computer, and can be run across a network or with remote display software, such as NX or Remote Desktop. It usually involves displaying both images on the screen simultaneously, and relies on focusing or simple devices to view the stereo effect. Hardware stereo requires some special equipment—a specialized monitor or graphics card, or both, and 3D glasses. It can usually only be viewed locally.

Two software stereo methods are available. In the first, two images are displayed simultaneously on separate parts of the screen, and the stereo effect relies on focusing your eyes so that

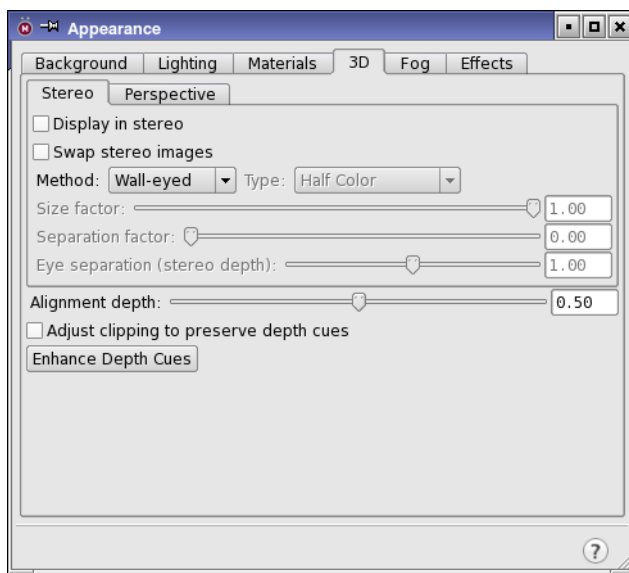


Figure 4.3. The Stereo tab in the Appearance panel.

the images appear to merge into a single image. Two variants of this method are available: “wall-eyed”, in which the left eye looks at the left image and the right eye looks at the right image (focusing at a very long distance); and cross-eyed, in which the left eye looks at the right image and the right eye looks at the left image (focusing at a very short distance). Neither of these variants needs any special hardware, though a device for screening out one image for each eye may be useful. The default variant is wall-eyed.

The second software stereo method is *anaglyph stereo*, in which the images are superimposed and are drawn with color filters, red and blue-green. To view the stereo effect, you need a pair of glasses with the appropriate color filter for each eye. The images have full color, but the red colors are not as true as when you do not view in stereo.

For hardware stereo, Maestro supports both quad-buffered hardware stereo and horizontally interlaced stereo. Details of the hardware and software requirements can be found in the [Installation Guide](#).

In quad-buffered stereo, the left and right images are displayed alternately on the screen. To reduce flickering, a monitor with a sufficiently high refresh rate is needed (better than 100 Hz).

In horizontally interlaced stereo, the left and right images are displayed on consecutive lines on the screen. The resolution is therefore not as high as for quad-buffered stereo, and text can be difficult to read. If the interlacing also alternates between left and right images each time the screen is refreshed (field-sequential interlacing), the synchronization with the glasses may be inverted. This can be fixed as described below.

To set the stereo viewing options, choose View → 3D Options in the main window and select the Stereo tab. To select a stereo viewing method, choose Wall-eyed, Cross-eyed, Interlaced, or Hardware from the Method option menu. To view the Workspace in stereo, select Display in stereo in the panel, or choose View → Stereo or press CTRL+S in the main window. These actions also turn off stereo viewing.

If you are using hardware stereo and the synchronization is inverted, select Swap stereo images. (This option also swaps cross-eyed and wall-eyed software stereo.)

If you are using the cross-eyed or wall-eyed method and the displayed stereo pairs are more than 2.5 inches from each other, adjust the Size factor, Separation factor, and Eye separation controls to bring the structures closer. This will make stereo viewing easier.

With any stereo method, you can adjust the eye separation and the alignment depth. Adjusting the eye separation changes the amount that the stereo image appears to extend into and out of the screen—the stereo depth—and adjusting the alignment depth makes the stereo image appear to move into or out of the screen. Decreasing the eye separation factor can help for interlaced stereo on some monitors.

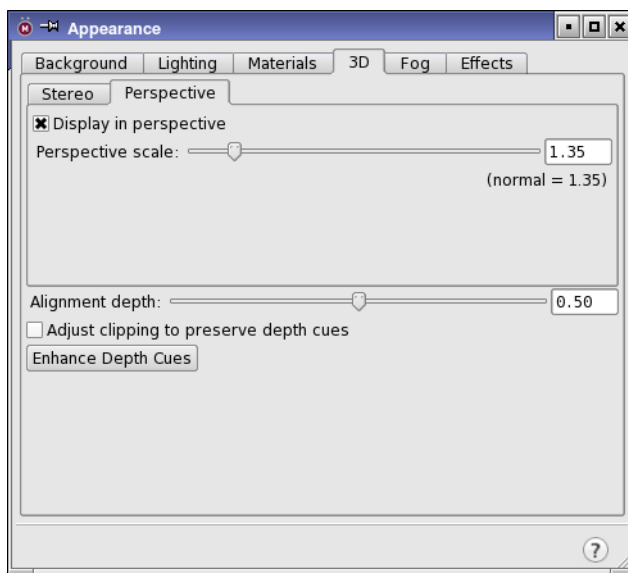


Figure 4.4. The Perspective tab in the Appearance panel.

The stereo method and stereo settings (size and separation) persist across Maestro sessions: they are saved in `prefer.cmd` in your profile directory.

### 4.7.2 Using Perspective

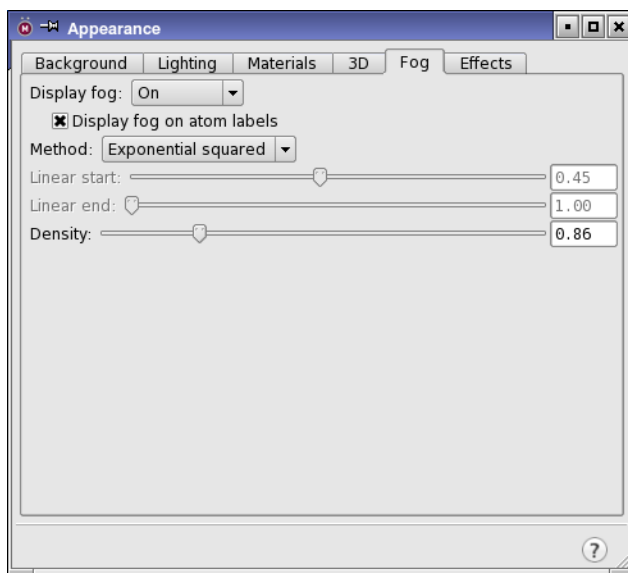
The Perspective feature enhances 3D graphical representation by scaling objects in the Workspace in proportion to their distance from the viewing plane (“camera”). Perspective is enabled by default. You can turn it on and off by choosing `View → Perspective`.

The perspective controls are in the Perspective subtab of the 3D tab. You can adjust the scaling using the Perspective scale slider. A larger value gives a stronger impression of depth (“depth cue”). The green lines in the Clipping Planes window move to reflect the viewing volume available at a given value on the Perspective scale.

### 4.7.3 Using Fogging

The Fog feature changes atom colors in the displayed structure so that they fade toward that of the background as atom coordinates grow increasingly negative in the  $z$  direction. This feature is particularly useful for depth-cueing when viewing large structures, such as proteins, and when using the Wire molecular representation.





**Figure 4.5.** The Fog tab in the Appearance panel.

The fog controls are in the Fog tab of the Appearance panel. To enable fogging, select On or Automatic from the Display fog option menu. You can independently apply fogging to atom labels using the Display fog on atom labels option. You can also turn fogging on or off from the Fog submenu of the View menu or from the Fog button menu on the Workspace toolbar.



Automatic fogging means that fogging is turned on when a molecule is bigger than a given number of atoms. Below this threshold, fogging is turned off. The threshold is 40 atoms, and can be set with the Maestro command `displayopt fogcutoff=number`.

The default method for fogging employs linear fall-off for the brightness of the displayed structural elements. To exaggerate the fogging effect, you can select either the Exponential method or Exponential squared method. When you are displaying a structure in perspective, you should use linear fall-off. The Automatic method uses linear fall-off with the start and end points determined by the background color.

The points at which fogging begins and ends can be controlled with the Linear start and Linear end sliders. Adjusting Linear start moves the boundary at which fogging starts between the front (0.0) and the back (1.0) of the displayed structure. Adjusting Linear end moves the fog boundary that is behind the structure further back, to a maximum of twice the depth of the

displayed portion of the structure. By adjusting these boundaries you can control the amount by which the structure appears to fade into the background.

For exponential and exponential squared fogging methods, the Density slider allows you to change the contrast of the colors used in fogging. Higher density makes closer portions of the structure appear brighter and more distant ones fade more quickly into the background.

Fog options are preserved between Maestro sessions.

### 4.7.4 Depth Cues

When you are viewing in stereo or in perspective and you zoom in on a structure, the structure can appear to “flatten”. This happens because the entire depth of the structure remains in the field of view when you zoom in: it is not clipped at all, and the depth cues (eye separation or perspective scale) are not preserved. You can preserve depth cues by selecting the Adjust clipping to preserve depth cues option. When you do this, the front part of the structure is clipped as you zoom in, so that you see only the parts of the structure that are “in front of you”, not the parts that are “behind you”.

The Alignment depth slider can be used to shift objects in or out of the screen, in order to change their relative size (depth scaling) or clipping.

The depth cues are affected by the location of the clipping planes: the closer they are to the structure, the better the depth cues. To move the clipping planes in to fit the displayed structure, click Enhance Depth Cues in the 3D tab, choose View → Fog → Enhance Depth Cues, press D in the Workspace, or click the Enhance button on the Workspace toolbar.



You can also enhance the perception of depth with the use of ambient occlusion. This feature is available for atom representations, and is set in the Atoms tab of the Molecular Representation panel. See [Section 7.3.1 on page 142](#) for details.

# Building and Adjusting Structures

Maestro provides a variety of tools for building and modifying structures. The Build toolbar and Fragments toolbar provide basic tools for building and modifying structures. In the Build panel, you can create molecular structures from a wide variety of predefined fragments and modify structures and properties of atoms and residues. The 2D Sketcher panel allows you to draw structures in 2D. Other panels enable you to add hydrogen atoms, adjust the geometry, connect or fuse molecules, and define centroids of groups of atoms. You can also set preferences for the behavior when certain building tasks are performed in the Preferences panel.

Some of the operations for building and modifying structures involve selection of atoms in the Workspace. For information on selecting atoms, see [Chapter 6](#).

## 5.1 The Build and Fragments Toolbars

The Build and Fragments toolbars provides quick access to tools for building, drawing, and modifying structures. To display these toolbars, choose Window → Toolbars → Build or Window → Toolbars → Fragments, or click the relevant button on the Manager toolbar.

The Build buttons are described below, and their use is described in detail later. For a description of the types of toolbar buttons, see [Section 2.4 on page 18](#).



### Draw structures

Enter Draw mode to draw structures freehand in the Workspace. Each click in the Workspace places an atom and connects it to the previous atom. The menu offers a choice of common elements for drawing (default C), and access to a periodic table for choosing other elements.



### Delete

Delete objects in the Workspace. The button menu has several sections: one for the current selection (DELETE), one for structural units to pick for deletion, one for other kinds of structural objects to delete, and one for markers and annotations. Double-click to delete the selected atoms.

Menu equivalent: Edit → Delete → Pick to Delete.



### Set element

Change the element for the atoms you pick in the Workspace to the element that is selected on the menu. The menu offers a choice of common elements (default C), and access to a periodic table for choosing other elements.



### Increment bond order

Increment the order of the bonds you pick in the Workspace by one, to a maximum of 3.



### Decrement bond order

Decrement the order of the bonds you pick in the Workspace by one, to a minimum of 0. Zero-order bonds are displayed with dashed lines (or tube segments).



### Increment formal charge

Increment the formal charge of the atoms you pick in the Workspace by one unit.



### Decrement formal charge

Decrement the formal charge of the atoms you pick in the Workspace by one unit.



### Invert chirality or flip ring substituents

Invert the chirality at a chiral center, or swap the substituents on an aliphatic ring atom, by picking the chiral center or the ring atom. Double-click to invert the chirality of all atoms.



### Move

Choose a direction for moving atoms, then click the atom to be moved. Moves in the XY plane are made by clicking the new location. Moves in the Z direction are made in 0.5 Å increments.



### Clean up geometry

Cleans up the geometry of the structure or the selected atoms in the Workspace by performing a short force-field minimization. You can choose the minimizer from the button menu: **Built-in** for the built-in minimizer using the OPLS\_2005 force field, and **UFF** for the universal force field minimizer, which covers more elements.



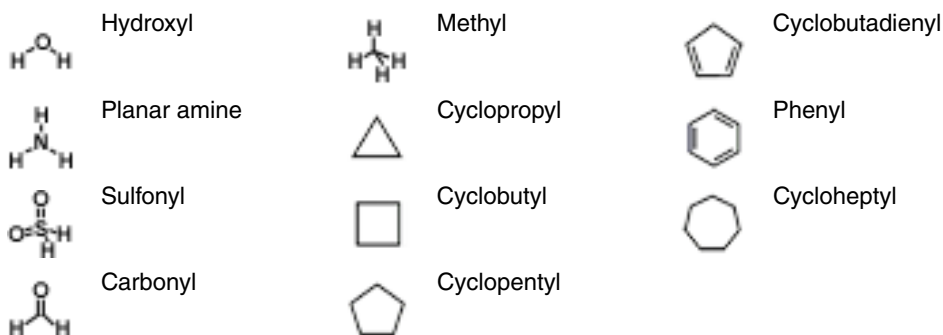
### Sculpt

Select and move atoms, followed by a short force-field minimization of the atoms in the same residue (or molecule). Atoms in residues within 5 Å are constrained, and the rest are frozen.

The set of fragment buttons on the Fragments toolbar provides a limited selection of structural fragments. These fragments can be added to the Workspace in Place mode (see [Section 5.3.1 on page 84](#) for details). The intention is that you build with these fragments to create the basic molecular framework, then change the element to introduce heteroatoms. A few specialized fragments with heteroatoms are provided, such as a planar amine fragment, which is useful for building amides. The fragment names are displayed in tool tips. A much larger set of fragments is available from the Build panel, which you can open by clicking the Fragments button:



The ring fragments can be attached by connection to an atom, which you do by picking an atom, or by fusion with a bond, which you do by picking a bond. The picking cursor is labeled A|B to indicate that either an atom or a bond must be picked.



In addition to the organic fragments, there is a button for placing metal centers, from which you can choose a metal center type, and place it in the Workspace.



The metal centers are also available in the Build panel. Once a metal center is placed, you must set the element for the metal center, as the metal is undefined (a dummy atom). By default, the attached ligand at each coordination site is hydrogen, but you can change it or replace it with a fragment or a metal ligand.

## 5.2 The Build Panel

The Build panel consists of three tabs. The primary building tools are contained in the Fragments tab. The Fragments tab contains several fragment libraries from which you can select a fragment and add it to the Workspace, either by positioning it manually or by using predefined grow rules. The other two tabs, Atom Properties and Residue Properties, contain tools for changing the properties of atoms or residues. The use of these tabs is described in the following sections.

To open the Build panel with a particular tab displayed, choose Edit → Build → *tab*, or choose the tab from the Build toolbar button menu on the Edit toolbar (if shown).



You can also open the Build panel at the Fragments tab with the Fragments button on the Fragments toolbar.



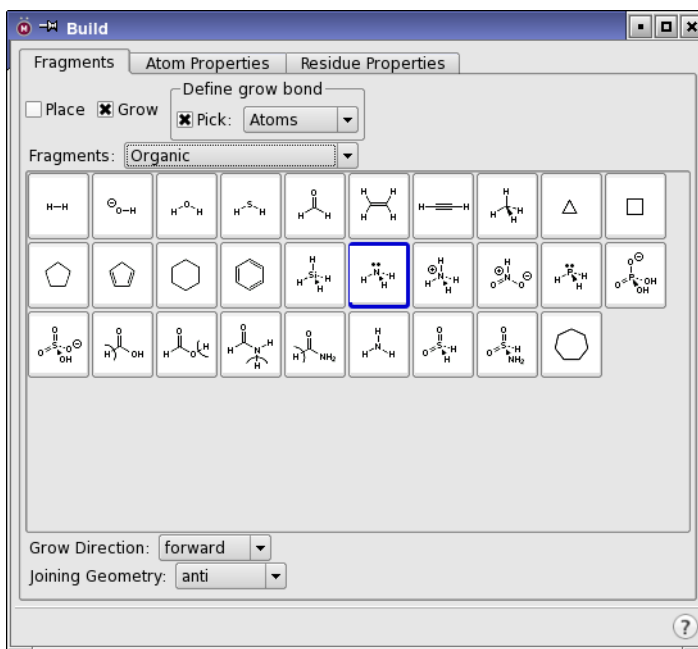
## 5.3 Building a Structure From Fragments

Whenever possible, you should use fragments to build structures. Building from fragments ensures the correct geometry within each fragment, and thereby reduces the work needed to minimize the structure. In addition to the small set of fragments on the Fragments toolbar, the following fragment libraries are available in the Fragments tab of the Build panel:

- Organic
- Rings
- N-heterocycles
- O-heterocycles
- S-heterocycles
- Mixed heterocycles
- Carbohydrate furanose
- Carbohydrate pyranose
- L carbohydrate furanose
- L carbohydrate pyranose
- Metal centers
- Metal ligands
- Amino acids
- Nonstandard amino acids
- Modified amino acids
- Protein capping groups
- Protein ions & solvents
- Deoxyribonucleic acids
- Ribonucleic acids
- Double-stranded A DNA
- Double-stranded B DNA
- Double-stranded A RNA
- Double-stranded B RNA
- Diverse fragments

These libraries are described briefly below.

- **Organic**—This library contains the common organic functional groups, a selection of simple ring structures, some common ions such as hydroxide, sulfate, nitrate, ammonium, and a hydrogen molecule.
- **Rings**—This library contains some more complex ring structures than those in the organic fragments library, including some fused ring structures, a basic steroid structure, porphyrin and phthalocyanine, buckminsterfullerene, and dodecaborane.
- **Heterocycles**—The four heterocycle fragment libraries provide a range of ring structures that contain nitrogen, oxygen, and sulfur atoms.
- **Furanose and pyranose structures**—Sugars can assume cyclized forms that include either five or six members. The five-membered ring form is called the furanose form, and the six-membered version is called the pyranose form. The natural state of most sugars is the pyranose form, but some derivatives assume a furanose form. Maestro provides both options in both D and L forms.
- **Metal centers and ligands**—These libraries contain common ligands used in inorganic chemistry and metal centers with various coordination numbers, but with the specific metal undefined. To change the metal type, retype the center once it is placed in the Workspace.



**Figure 5.1.** The Fragments tab of the Build panel, showing the Organic library.

- **Amino acids**—The Amino acids library contains the 22 naturally-occurring amino acids. The Nonstandard amino acids library includes the D forms of the 22 naturally-occurring amino acids and various other residues. The Modified amino acids library includes the five residues MSE (selenomethionine), ASQ (phosphoaspartate), TPO (phosphothreonine), PTR (phosphotyrosine), and SEP (phosphoserine).
- **Protein capping groups**—This library contains some common molecules used to cap peptides.
- **Protein ions & solvents**—This library contains common solvents and solvent ions found in protein structures, and is primarily intended for placement of these species in PrimeX. These fragments cannot be used for growing because they do not have designated grow bonds.
- **Nucleic acids**—The Deoxyribonucleic acids library contains Adenosine, Cytosine, Guanine, and Thymine, while the Ribonucleic acids library contains Adenosine, Cytosine, Guanine, and Uracil. The double-stranded DNA libraries contain deoxyribonucleic and ribonucleic acid base pairs in the A and B helix formations.
- **Double-stranded DNA and RNA**—These four libraries provide the fragments for building DNA and RNA in the A and B helix conformations.

- **Diverse fragments**—This is a collection of chemically diverse fragments with chains of various lengths attached to the main functional group. It is useful for examining structure-activity relationships. It is intended for use with MCPRO+ for free-energy perturbation calculations of relative ligand binding energies.

To select a fragment library, choose the library from the Fragments option menu. The area below this menu contains a grid of buttons that you use to select fragments. Each button displays either the name of the fragment, an abbreviation for the fragment name, or the fragment structure. If a structure is displayed, the name of the fragment is given in the Balloon help for the button.

If the particular fragment you want to use is not in the supplied libraries, you can build it from other fragments, or select a fragment with a geometry similar to the one you want to use, then replace atoms with those of different elements from the Atom Properties tab.

The fragment libraries and grow rules are read and interpreted at run time. If you are interested in creating your own fragments or fragment libraries, please write to [help@schrodinger.com](mailto:help@schrodinger.com) to obtain the appropriate instructions.

### 5.3.1 Building Structures Using Place Mode

You can use Place mode to create multiple molecular structures in the Workspace, to assemble structures from multiple fragments, and to change a fragment into another fragment within a structure. Place mode is the mode in force when you use the Fragments toolbar to build structures. To enter Place mode when using the Build panel, select Place in the Fragments tab.

To create multiple structures in the Workspace in Place mode, select a fragment from the build toolbar or choose a library from the Fragments option menu in the Build panel and select a fragment, then click in the Workspace. Repeat this process, clicking in a different place in the Workspace for each new fragment you want to place. The fragments are placed in a predefined orientation at the location you select, and are completed with hydrogen atoms to form molecules. If you now want to join these structures to form a single molecule, you can use the tools in the Connect/Fuse panel. See [Section 5.8 on page 97](#) for details.

When you build a structure from fragments, a new project entry is automatically created, with the default title Structure*N*. You can edit the title of the entry to change it. If the Workspace contains a single entry when you start building, placing a fragment that is not connected to the structure in the Workspace, adds the new fragment to the Workspace entry. This means that placing multiple fragments will put all these fragments into a single project entry. If there are two or more project entries in the Workspace, you are prompted to choose an entry to add the fragment to, or to create a new entry. Each new fragment you place in these circumstances will produce a prompt, so it is best to start placing fragments in an empty Workspace or one with only one entry.



You can build a single structure from multiple fragments in Place mode. Once you have placed the first fragment, you can join a second fragment to it by selecting the fragment and clicking in the Workspace on the atom that you want the new fragment to replace. If you click on a terminal atom, the fragment replaces the terminal atom. If you click on a non-terminal atom, that atom and its attached hydrogen atoms are replaced by the new fragment. For example, clicking on a secondary amine nitrogen with a methyl fragment gives a disubstituted methyl center, and clicking on a disubstituted methyl carbon with an amine fragment produces a secondary amine center.

If you are using the build toolbar to add a ring to a structure, you must ensure that you are in connection mode (A cursor label) rather than fusion mode (B cursor label). Clicking on the ring button switches between the modes.

You can also mutate one residue into another in a protein. When you select Amino acids or Modified amino acids from the Fragments menu in the Build panel, a Mutate button appears beside the Define grow bond picking tools. To mutate a residue, select Mutate, select the new residue from the list and pick an atom in the residue you want to mutate. The new residue replaces the old residue. A quicker way of mutating a residue is to right-click on an atom in the residue and choose the new residue from the Mutate Residue submenu of the shortcut menu that is displayed.

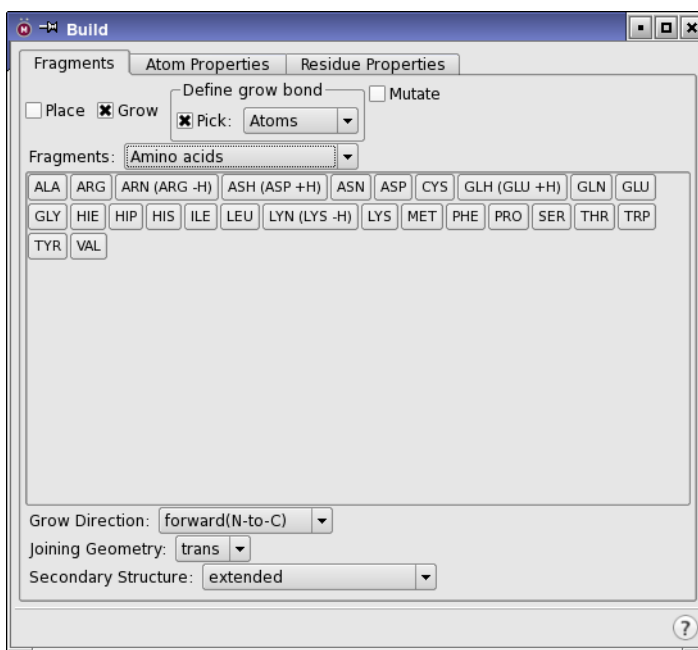


Figure 5.2. The Fragments tab of the Build panel, showing the Mutate option.

### 5.3.2 Building Structures Using Grow Mode

In Grow mode you can take advantage of the predefined “grow” rules that dictate where and how fragments are connected to build structures. To enter Grow mode, select Grow in the Fragments tab of the Build panel. This mode is only available from the Build panel.

To create a structure in Grow mode, click the fragments in the fragment library that you want to assemble in the Workspace. At each click, the selected fragment is added to the structure, and a green arrow marks the location of the *grow bond*—the bond that will be replaced when the next fragment is added.

To grow a structure from a location other than that indicated by the current grow bond, you can choose a new grow bond using one of the following methods:

- Choose Atom from the Pick option menu of the Define Grow Bond section, and pick two atoms in the order that defines the grow direction.
- Choose Bond from the Pick option menu of the Define Grow Bond section, and pick a bond. The grow direction arrow points to the atom closest to where you click.
- Choose backward from the Grow Direction option menu. The grow bond moves to the opposite end of the molecule.

In addition to the fragments, the Fragments tab of the Build panel contains controls for setting the joining geometry, and, where applicable, secondary structure and helix geometry. The Joining Geometry option menu provides context-sensitive options for attaching new fragments to the existing structure. For example, under the Deoxyribonucleic acid fragment type, the joining geometry options are Standard Helix and User Defined.

If you choose to define your own joining geometry, you must specify values for the torsions that define applicable secondary and tertiary structures. When you select the User Defined option and click on the name of the fragment, a dialog box prompting you to enter the angle value is displayed.

If you are growing a structure with amino acid fragments, and you choose user defined from the Secondary structure option menu, you are prompted for the phi angle and then the psi angle. When growing in the N→C direction, the phi angle is applied to the new residue, but the psi angle is applied to the residue that the new residue is attached to. This is because the N–C bond is replaced when you grow the next residue; the new residue always has psi set to 180°.

By default, Maestro automatically fits the structure to the Workspace after each grow operation. You can turn this behavior off in the Builder tab of the Preferences panel (see [Section 14.11 on page 365](#)).

When growing residues (amino acids, DNA/RNA, sugars—any fragment that has a residue name), the residue number is incremented or decremented from the number of the residue that you grow from, depending on the direction of growth, and the new residue is assigned the same chain name. For other fragments (that don't have a residue name), the added fragment inherits the chain name and residue number of the residue it was attached to by the grow operation.

## 5.4 Building a Structure From Atoms

The Build toolbar contains tools for drawing structures in the Workspace atom by atom (Draw mode), and the Atom Properties tab and the toolbar contain tools for retyping atoms within a structure. Maestro does not automatically correct geometries of structures created in Draw mode. You can adjust the geometry after building the structure from the Adjust panel. You should also minimize the energy of the completed structure.

When using Draw mode to create a structure, only a few elements—H, C, N, O, P, S, Si, Al, Cl, and F—are available by default on the button menu. You can use other elements by choosing Other from the button menu and selecting the element from the periodic table in the element selector that opens. Alternatively, you can use one of the common elements to draw the structure, and then change the desired atoms—see [Section 5.6](#). Maestro allows you to violate the valency of an atom in Draw mode so that you can change it to an atom of some other element.

The basic operations of Draw mode are described below.

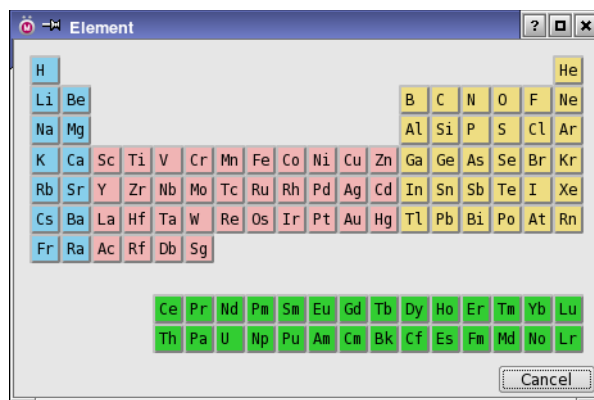
- To begin drawing with the currently selected element, click the Draw button.



The Draw structures button appears indented, indicating that you are in Draw mode. The default element is carbon.

- To place an atom, click in the Workspace.

The atom appears as an asterisk enclosed in a purple cube. The cube marks the “active” atom, which means that it is automatically bonded to the atom that is placed next. Each subsequent click in the Workspace places another atom and bonds it to the previous atom with a single bond. To finish drawing, click the active atom. The cube vanishes.
- To start drawing from another location in the structure, deactivate the active atom by clicking on it, then click on the atom that you want to start drawing from. This atom becomes the active atom.
- To connect the active atom to an existing atom, click the existing atom.



**Figure 5.3. The element selector.**

- To create a multiple bond between the active atom and an adjacent atom, click the adjacent atom. Another bond is added between the two atoms.
- To change the element that you are drawing with, choose the element from the Draw button menu, or choose Other and select it in the element selector. The next new atom you place will be an atom of the new element. If you connect existing atoms of a different element, the element of the existing atom is not changed: thus, it does not matter which element is selected when you draw a bond between two existing atoms.

The atoms that you draw are placed in the  $xy$  plane (the plane of the screen). If you want to create a 3D structure, you can rotate the structure in the Workspace with the middle mouse button, then continue drawing atoms. Rotation does not change the active atom or exit Draw mode. You can also move atoms that you have placed using the Move button menu.



To move an atom in the  $xy$  plane, choose X-Y from the button menu, click the atom you want to move, then click the new location. If the atom is in a ring, only the atom is moved. If the atom is not in a ring, the atom and its attached atoms are moved. To move an atom in the  $z$  direction, choose +Z or -Z from the menu, and click the atom to be moved. The atom is moved 0.5 Å in the chosen direction.

## 5.5 Building a Structure in 2D

Draw mode (Section 5.4) allows you to build a structure in 3D by drawing in the Workspace. Maestro offers another tool, for sketching structures in 2D. The structures can be saved as project entries, either with 2D coordinates, or converted to 3D with LigPrep. 2D structures can be sketched in the 2D Workspace panel, which you open by choosing Edit → 2D Sketcher, or clicking the Sketcher button on the Edit toolbar.



The 2D Sketcher dialog box has a menu bar at the top, a drawing area, a toolbar to the left of the drawing area, and options for creating a project entry below the drawing area.

### 5.5.1 The 2D Sketcher Menu Bar

The menu bar has three menus: File, Edit, and View. The File menu has a single item, Save Screenshot, which saves an image of the drawing area in a file. The image can be saved in PNG, JPG, or BMP format. The shortcut key is CTRL+ALT+P (⌘P).

The Edit menu has the usual Undo (CTRL+Z, ⌘Z) and Redo, Copy (CTRL+C, ⌘C) and Paste (CTRL+V, ⌘V) items. Copy copies the selected atoms or the entire structure to the clipboard as a SMILES string. Paste places the SMILES string in the center of the display area as a 2D structure. Select All (CTRL+A, ⌘A) and Deselect (CTRL+D, ⌘D) select all atoms and clear the selection. Cleanup cleans up the structure (2D coordinates) and normalizes the orientation and arrangement of groups.

The two remaining items on the Edit menu allow you to get structures from other sources:

- Input SMILES String (CTRL+S, ⌘S) allows you to add a structure to the center of the drawing area by specifying its SMILES string in a dialog box.
- Common or IUPAC Name Search (CTRL+P, ⌘P) allows you to run a PubChem query (on the web) on the common name or IUPAC name of a structure that you provide in a dialog box. The first result is added as a 2D structure to the center of the drawing area.

The View menu has items for flipping the structure, zooming in or out, changing the background, and labeling or coloring atoms. Flip Vertical (CTRL+ALT+F, ⌘F) flips the structure from top to bottom, and Flip Horizontal (CTRL+ALT+H, ⌘H) flips the structure from left to right. Fit to Screen (CTRL+F, ⌘F) zooms in or out so that the structure fills the visible part of the drawing area. If you prefer to see the structure in white on a black background, like on a blackboard, choose Blackboard View (CTRL+I, ⌘I). Finally, choose User defined fragments to show or hide the User-defined fragments toolbar.

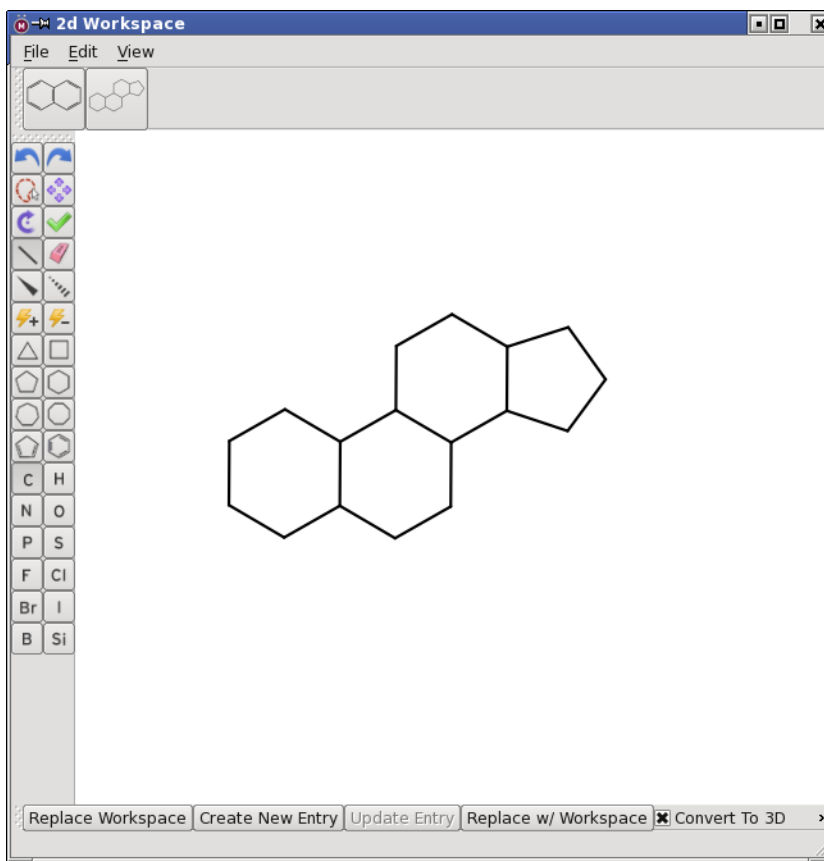














Figure 5.4. The 2D Sketcher panel.

You can label chiral atoms with R or S by choosing Stereochemistry Labels (CTRL+L, ⌘L), and you can color atoms other than carbon by choosing Color Heteroatoms (CTRL+T, ⌘T). N is blue, O is red, S is yellow, and so on.

### 5.5.2 The 2D Sketcher Toolbar

The toolbar has three sets of buttons. The first set of buttons is for performing actions, which are described below. The second set is a collection of rings that you can add to the structure. The third set is a collection of elements, which you can use to change atoms to a chosen element. The selection of the element can also be done by typing the element symbol (case insensitive).

-  **Undo**  
Undo the last action. Can be performed multiple times.
-  **Redo**  
Redo the last action that was undone. Can be performed multiple times.
-  **Lasso**  
Select atoms by drawing around them (“lassoing”). The selected atoms can be moved, rotated, deleted, copied.
-  **Move**  
Move (translate) the selected atoms or the entire structure. Drag in the drawing area to move the structure. Drag the selection to move the selected atoms. (This is the default action for dragging a selection, so you do not need to click this button before dragging it.) You can also move the structure by dragging with the right mouse button.
-  **Rotate**  
Rotate the selected atoms or the entire structure. Drag in the drawing area to rotate the structure. The angle through which the structure has been rotated is displayed near the center of rotation while you are rotating it. If rotation does not seem to be working properly, check whether you have other structures in the drawing area that are not visible. You can also rotate the structure by dragging with the middle mouse button.
-  **Cleanup**  
Clean up the structure (2D coordinates) and normalize orientation and arrangement of groups. If you have atoms selected, only those atoms are cleaned up.
-  **Draw**  
Draw a single bond. Click on an atom to draw a bond to a new (carbon) atom, click on a bond to add another bond between two atoms.
-  **Erase**  
Delete atoms or bonds. Clicking on a carbon atom deletes it; clicking on a non-carbon atom changes it back to carbon, then clicking again deletes it. Clicking on a bond removes one bond.
-  **Wedge Bond**  
Draw a wedge bond. Clicking on an atom draws a wedge bond to a new (carbon) atom; clicking on a single bond converts it to a wedge bond.
-  **Dashed Bond**  
Draw a dashed bond. Clicking on an atom draws a dashed bond to a new (carbon) atom; clicking on a single bond converts it to a dashed bond.
-  **Increase Charge**  
Increase the formal charge on an atom by 1.
-  **Decrease Charge**  
Decrease the formal charge on an atom by 1.

### 5.5.3 Sketching Molecules

To start drawing, click the Draw button.



Drawing creates a carbon-atom framework. You can change the element with the element buttons, either during drawing or after you have finished drawing, or by typing the element symbol while the pointer is over an atom.

The first atom is placed by clicking in the drawing area. It is shown as CH<sub>4</sub>. After placing the first atom, you can draw in several ways:

- Click on an atom to place a new atom and draw a bond to it from the clicked atom. The bond is placed in a default orientation with respect to existing bonds.
- Drag from an atom in a particular direction, to place a new atom and draw a bond from the clicked atom to the new atom in the chosen direction.
- Drag from an atom to another atom to create a bond between the two atoms.
- Hold down shift and drag from an atom to add a linear chain to that atom.
- Click on a bond to increase its bond order.

The “active” atom—the one to which a new bond will be attached—is indicated by a gray filled circle. Likewise, the active bond is indicated by a thicker gray line. The active atom or bond changes as you move the pointer over the atoms or bonds.

You can also start your drawing with a ring: click on the ring in the toolbar then click in the drawing area to place the ring.

To draw bonds with a given stereochemistry, click the Wedge Bond or Dashed Bond button,



and draw in the drawing area. Clicking on a bond changes its stereochemistry; clicking on an atom adds a new atom with the selected orientation.

To add rings to your system, click on one of the ring buttons, then click in the drawing area. When you move the pointer into the drawing area, the ring is shown in blue. As you move the pointer in the drawing area, the ring “snaps” to positions that show a potential attachment of the ring to the structure. Clicking when the ring is in one of these positions places the ring at that position, and its color changes to black. You can do the same with the fragments on the User-defined fragments toolbar.



To add a functional group, pause the pointer over the atom you want to add the group to, then type – followed by its name, and press ENTER, e.g. -et to add an ethyl group. Many common functional groups are recognized: the list is given in Table 5.1 with the corresponding SMARTS patterns; the names are case-insensitive. You can also replace an atom with a functional group, by omitting the initial –.

Table 5.1. Functional group names and SMARTS patterns for use in editing 2D structures.

Name	SMARTS	Name	SMARTS	Name	SMARTS
me	C	ph	C(C=C1)=C-C=C1	coo-	C(=O)[O-]
et	CC	bz	CC(C=C1)=C-C=C1	no2	[N+](=O)[O-]
pr	CCC	chex	C(CC1)CCC1	so2	S(=O)=O
ipr	C(C)C	cp	C(C=C1)C=C1	so2n	S(=O)(=O)N
nbu	CCCC	ome	OC	so3	S(=O)(=O)[O-]
ibu	CC(C)C	oet	OCC	po3	P(=O)([O-])[O-]
sbu	C(C)CC	cooh	C(=O)O	con	C(=O)N
tbu	C(C)(C)C	coome	C(=O)OC	nco	NC=O
nhex	CCCCCC	cooet	C(=O)OCC	cn	C#N

To change the element, you can do one of the following:

- Pause the pointer over the atom, then type the element symbol.
- Click the button for the desired element on the toolbar, then click an atom in the structure.
- Type the element symbol, then click an atom in the structure.

The last two of these choices allow you to click on multiple atoms to change the element; the first operates only on the active atom.

To assign a formal charge, click the Increase Charge button or the Decrease Charge button,



then click on an atom. The formal charge is given next to the atom, and any hydrogens are also shown that are needed to complete the valence for the atom; or a red underline is shown to indicate that the valence is not satisfied. You can also pause the pointer over an atom and type in the formal charge. Any combination of numbers, +, and – is accepted.

To move a group, first select the group by drawing around it with the Lasso tool:



If you want to translate it, just drag it to the new location. The pointer must be over the group when you start to drag it. If you want to rotate it, click the Rotate button,



then drag it to the new orientation. As for translation, the pointer must be over the group when you start to drag it. The angle is displayed as you drag.

To adjust the view, you can zoom in or out with the scroll wheel or pinch gesture, pan (translate) with the right mouse button, and rotate with the middle mouse button.

### 5.5.4 Saving Templates for Building

You can save structures as templates that you can use to build other structures. These templates are displayed on the User-defined fragments toolbar, which you display by choosing View → User defined fragments. When you have drawn a structure that you want to add to the toolbar, press CTRL (⌘) and drag the structure to the toolbar. A new button is added with the structure displayed on it. To remove a structure from the toolbar, click on the button and press DELETE or BACKSPACE. You can use these fragments in the same way as the ones on the main toolbar.

### 5.5.5 Saving Structures

You can save a structure as a project entry in several ways, with the buttons at the bottom of the panel:

- **Replace Workspace**—Replace the Workspace with the sketched structure, as a scratch entry.
- **Create New Entry**—Create a project entry from the structure in the drawing area. A default title is assigned to the entry. Hydrogens are added to the structure; it is converted to 3D if Convert to 3D is selected.
- **Update Entry**—Update the project entry from which the structure was taken with the updated structure in the drawing area. Hydrogens are added to the structure; it is converted to 3D if Convert to 3D is selected.

If you have a LigPrep license, you can convert it to 3D by selecting Convert to 3D; otherwise it is added as a 2D structure, and you must convert it to 3D if you want to use it for calculations. Hydrogens are always added when saving a structure as a project entry.

To save an image of the structure in PNG, JPEG, or BMP format, press CTRL+ALT+P. A dialog box opens with controls for the size of the image and an option for saving with a transparent background. When you click OK, a file selector opens, in which you can navigate to the location and name the file. The image type is determined by the file extension.

## 5.6 Changing Elements

Whether you build a molecule in Place mode, Grow mode, or Draw mode, the range of elements available to you by default is limited. Even with access to the whole range of elements, it is often more efficient to quickly sketch a structure as a carbon skeleton and then change the elements to the desired ones afterwards. You do not have to complete the structure before you make the change, you only have to place an atom at the desired location.

Changing an atom from one element to another can be done from the Build toolbar, the Selection shortcut menu, or from the Atom Properties tab.

From the Set Element button menu on the Build toolbar you can choose H, C, N, O, P, S, F, Cl, Br, I, Al, or Si, then click on an atom in the Workspace to change it to the selected element.

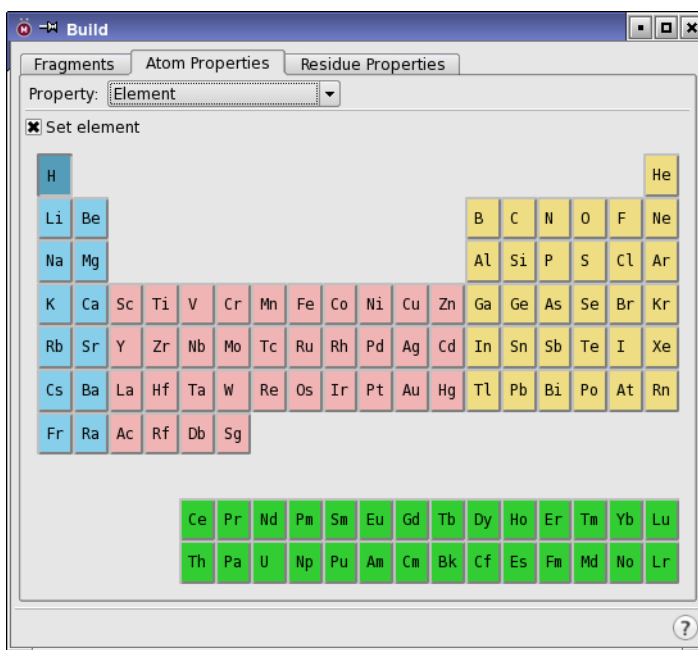


Figure 5.5. The Atom Properties tab showing tools for the Element property.

To change to other elements, you can choose **Other** on the button menu and select an element in the element selector (see [Figure 5.3 on page 88](#)). The element is listed in parentheses after **Other** on the button menu, to indicate that it is the current element.

To use the shortcut menu, select the atoms to change, then right-click in the Workspace and choose **Set Element**, then choose the element. The same range of elements is available as on the toolbar button, and also the **Other** item for choosing other elements.

To use the **Atom Properties** tab in the **Build** panel, first choose **Element** from the **Property** menu. A periodic table is displayed, from which you can select an element, then click on an atom in the Workspace to change it to that element. You do not need to select **Set Element**: this is done automatically when you click on an element in the periodic table. However, you can select **Set Element** if it is unselected and you want to use the currently selected element.

## 5.7 Changing the Bond Order and Formal Charge

After creating a structure, you may wish to change some of the bond orders or formal charges. You can make these changes with the tools on the **Build** toolbar (as shown below) or by right-clicking a bond and choosing the appropriate item from the shortcut menu.

- To increase the bond order, click the **+ Bond Order** toolbar button



then click the bonds whose order you want to increase. Each click increments the bond order by one, up to a maximum of three. You can also increase the bond order in **Draw** mode by drawing another bond between the two atoms.

- To decrease the bond order, click the **- Bond Order** toolbar button



then click the bonds whose order you want to decrease. Each click decrements the bond order by one, to a minimum of 0. Zero-order bonds are displayed with dashed lines in wire representation and tube segments in tube representation.

When you change the bond order, the valence states of the atoms can be violated. Maestro gives no warning of this violation, so it is up to you to ensure that your structure is valid.

- To increase the formal charge, click the **+ Formal Chg** toolbar button



then click the atoms whose formal charge you want to increase. You can only increase the formal charge one atom at a time. However, the formal charge is also set when you change the MacroModel atom type.

- To decrease the formal charge, click the - Formal Chg toolbar button



then click the atoms whose formal charge you want to decrease. Like increasing the formal charge, you can only decrease the formal charge one atom at a time, and the formal charge is set when you change the MacroModel atom type.

## 5.8 Connecting or Fusing Structures

To build some structures, it is sometimes convenient to connect or to fuse two existing structures. Connecting two structures creates a new bond between two selected atoms, with deletion of appropriate hydrogens. An example is the creation of bipyridyl from two pyridine rings, by connecting the 2-carbon on one ring with the 5-carbon on the other, and deleting the hydrogen atoms. Fusing two structures deletes atoms. An example is the fusion of two benzene rings, in which two carbon and two hydrogen atoms are deleted from one ring, and bonds formed to the other ring with deletion of two hydrogen atoms, to form naphthalene.

Fusion of rings can be accomplished when building structures using the Build toolbar. Each ring fragment can be fused onto the existing structure by clicking a bond.

You can connect structures with draw mode, by clicking on the two atoms you want to connect. However, no adjustment of the geometry is made when you do so.

More general tools for fusing and connecting structures are available from the Connect and Fuse panel, which you open from the Edit menu. The panel is docked into the Workspace by

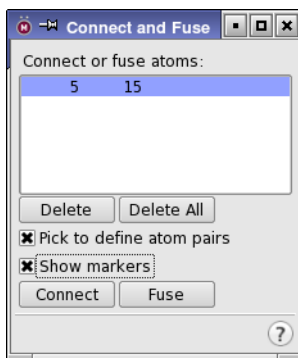


Figure 5.6. The Connect & Fuse panel.

default, but you can move it out. In the connection and fusion operations, an attempt is made to create structures with reasonable geometries, and a check is made that valency is not violated. This is in contrast to Draw mode, which does not evaluate bonding or geometry.

For both connect and fuse operations, you must first select atom pairs to be joined. The atoms you select must not be hydrogen atoms. You can select as many pairs as you like. The first atoms in all selected pairs must all come from the same molecule, and the second atoms in the pairs must come from the same molecule. The molecule for the set of first atoms set need not be different from the molecule for the set of second atoms. If you select a pair of atoms in the same molecule, a new bond is drawn between the atoms.

To select atoms for a connect or fuse operation, ensure that **Pick to define atom pairs** is selected and click on the Workspace atoms to define the pairs. Atom numbers of the selected pairs appear in the Connect or fuse atoms list. Also, if **Show Markers** is selected, each pair is marked with a dashed green line. For the pair that is selected in the list, the green line is flanked by solid yellow lines. The lines disappear once the connect or fuse operation is completed.

When fusing structures, the order in which you select the atom pair is important. The first atom selected is replaced by the second atom selected. For example, when fusing an amino nitrogen and an ethyl carbon, selecting the nitrogen first results in its deletion, followed by attachment of the remaining atoms of the amine to the ethyl carbon. Selecting the ethyl carbon first results in deletion of the carbon and retention of the nitrogen.

To delete an atom pair from the Connect or Fuse Atoms list, select the pair in the list and then click **Delete**. To clear the atom pair list, click **Delete All**.

When you have selected all the pairs of atoms that you want to connect or fuse, click the appropriate button—**Connect** or **Fuse**.

If you are performing a connection or fusion between structures belonging to different project entries (the source entries), the result must belong to a single entry. When you click **Connect** or **Fuse**, the **Choose Entry** dialog box opens, and you must specify the entry with which the new structure should be associated. Subsequent actions depend on which entry you choose:

- If you choose one of the two source entries, the other entry is deleted.
- If you choose an existing entry other than the two source entries, the new structure is added to the existing entry and the source entries are deleted.

When you draw a bond between two entries, a new entry is created automatically, and you can name the new entry in the **Create Bond** dialog box. If one of the entries is a scratch entry and the other is a project entry, the scratch entry atoms are added to the project entry and the scratch entry is deleted. If both entries are scratch entries, they are merged into one of the scratch entries and the other is deleted.

You can undo a connect or fuse operation, and the changes to the entries are also undone.

## 5.9 Adjusting the Geometry

Before you use a structure for a calculation, you might want to adjust the geometry, especially if you used Draw mode, or if the Grow mode orientation was incorrect. Maestro provides tools on the Edit toolbar for the most common adjustments, on the Adjust button menu.



More flexibility is provided in the Adjust panel, which you open from the Adjust submenu of the Edit menu in the main window. The tools that are available on the Adjust button menu are also available from the Adjust submenu of the Edit menu.

### 5.9.1 Adjusting Distances, Angles, and Dihedral Angles

You can change distances, angles, and dihedral angles, either directly in the Workspace or by using the tools in the Adjust panel, as described below. If you are making a sequence of adjustments of the same type, you can easily recall the previous or next adjustment.

#### 5.9.1.1 Using the Workspace Tools

The basic process for adjusting parameters directly in the Workspace is the same for distances, angles, dihedral angles, and chirality. This description uses distances as an example:

1. Choose Distance from the Adjust button menu on the Edit toolbar:



2. In the Workspace, click on two atoms to define the distance.

A purple cube is drawn around the first atom, to indicate that it has been selected. For angles and dihedrals, a cube is drawn around each subsequent atom.

When you click the last atom, the distance is highlighted with two yellow solid lines, a purple dotted line, and an arrow indicating the direction of adjustment. Angles are highlighted in green and orange, and dihedrals are highlighted in red and turquoise.

3. With the left mouse button, drag to the right to increase the distance or to the left to decrease it. Alternatively, use the scroll wheel or the pinch gesture to adjust the distance.

You can choose bond lengths or dihedrals for adjustment by right-clicking on a bond in the Workspace and choosing Distance or Dihedral from the Adjust submenu on the shortcut menu.

For a faster adjustment of a dihedral, choose Quick Torsion from the Adjust button menu, click on a bond, then drag with the left mouse button. The fragment that is rotated has an arrow pointing to it on the end of the bond nearest the moving fragment. By default the smaller fragment is rotated around the selected bond. To change the fragment that is rotated, click the bond again. Quick Torsion is selected by default, so if you have not previously selected some other adjustment, you only need to click on the Adjust button, then perform the adjustment.

If you want to display interactions such as hydrogen bonds and contacts while adjusting structures, you can select Display Interactions from the Adjust button menu. The interactions that are displayed can be set as preferences—see [Section 14.8.2 on page 360](#) for more information.

### 5.9.1.2 From the Adjust Panel

The tools for adjusting bond lengths, bond angles, and dihedral angles are similar, so the description given here is generic.

To define the geometric parameter that you want to adjust, choose Atoms or Bonds from the Pick option menu in the Define atoms for *operation* section, and pick the atoms or bonds. For a bond length, you must pick two atoms or one bond; for a bond angle, you must pick three atoms or two bonds; for a dihedral angle you must pick four atoms or one bond—the bond about which the rotation is performed. When you pick this bond, the groups attached to the atom nearest the point you click are the ones that are moved.

In addition to the standard picking tools just described, you can also specify dihedrals in proteins using standard names (psi, phi, omega, etc.). Click Select in the Dihedral tab and select dihedrals by the residues in each entry (or chain), or by standard names.

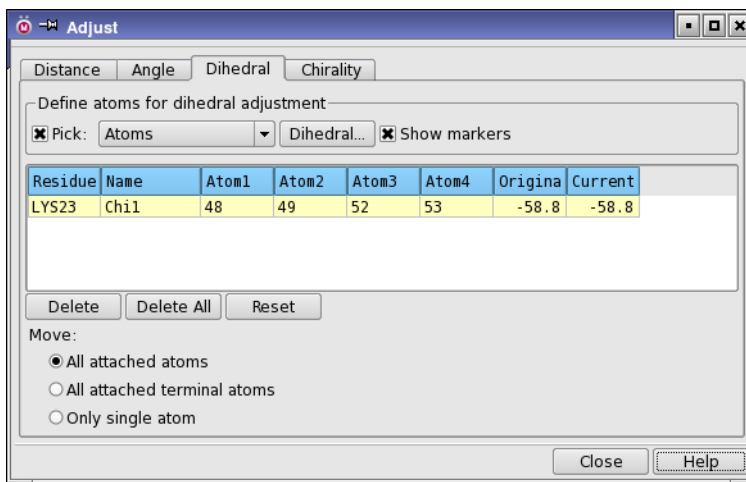


Figure 5.7. The Adjust panel, showing the Dihedral tab.



The atom numbers of the selected atoms are listed in the table in the center of the tab. The last atom that you pick is the “target atom”—the atom that is moved in the adjustment process. You must also decide which of the attached atoms to move along with the target atom. You can choose from All attached atoms, All attached terminal atoms, or Only single atom. If the target atom is part of a ring, the first option is unavailable.

Once you have chosen the atoms for a particular adjustment, you can make the adjustment by dragging with the left mouse button, by using the scroll wheel, or by entering a new value for the geometric parameter in the Current column of the table. If you enter a new value, the value is changed and the Workspace is updated when you press ENTER. You can make adjustments using the table at any time, but you can only use the mouse immediately after picking.

### 5.9.1.3 Repeating Adjustments

When adjusting a structure, you might want to switch between adjusting two or more parameters. If the parameters are of the same type, you can select the previous or the next adjustment by choosing Edit → Adjust → Previous Adjustment or Edit → Adjust → Next Adjustment, or use CTRL+SHIFT+A (⌘Z) and CTRL+SHIFT+Z (⌘Z). If they are of different types, you can select the adjustment type again, using the Edit menu or the Adjust button, and the last adjustment of that type made is selected. You can also select the adjustment you want to change in the Adjust panel, by selecting the table row in the tab for the adjustment type.

## 5.9.2 Adjusting Peptide Linkages and Side Chains

The Adjust button menu on the main toolbar provides some tools for adjusting the geometry of peptide linkages, and for selecting the most common rotamers for side chains.

For peptide linkages, you can rotate the plane of the peptide linkage, rotate the carbonyl plane, and convert between cis and trans linkages.

### To perform peptide rotations:

1. Choose Rotate Peptide Plane or Rotate Carbonyl Plane from the Adjust button menu on the Edit toolbar.



2. Click on an atom in the peptide group to select it.

The peptide group is marked with a rectangle.

3. Drag with the left mouse button to perform the rotation.

**To convert between cis and trans:**

1. Choose Convert Cis/Trans from the Adjust button menu on the Edit toolbar.
2. Click on one of the atoms in the peptide link.

The geometry of the converted link is only approximate, and should be refined before use in any application that depends on the accuracy of the geometry.

**To select a rotamer for one or more residue side chains:**

1. Select the residues in the Workspace or the sequence viewer.
2. Choose Rotamers from the Adjust button menu on the main toolbar.

The Rotamers dialog box opens. This dialog box has a list of the residues you selected in the Workspace at the top and a list of rotamers for the residue that is selected from this list below, with angles and a standard percentage population for each rotamer.

3. Select a residue from the table at the top of the dialog box.

The residue is highlighted in the table. The Workspace view zooms to that residue if Fit selected residue to Workspace is selected.

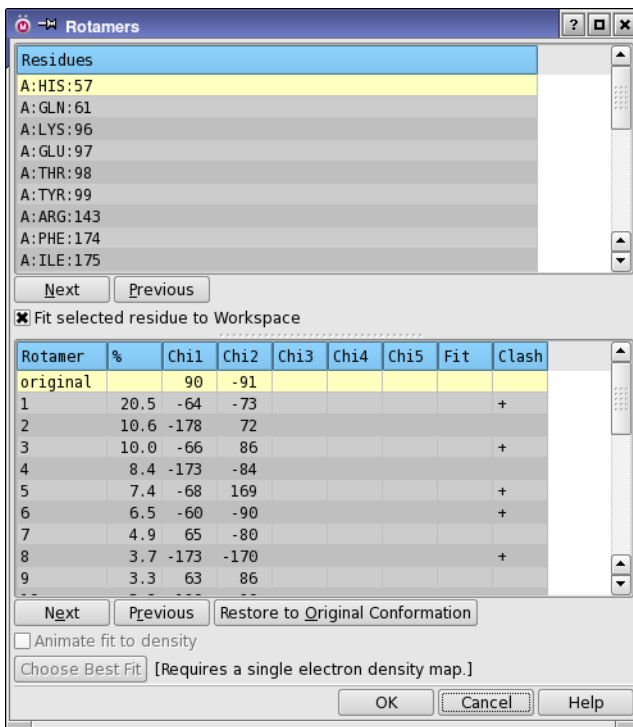


Figure 5.8. The Rotamers dialog box.

4. Select a rotamer from the lower table.

The side chain is rotated to the geometry of the selected rotamer. You can sort this table by clicking on the column headings.

Repeat steps 3 and 4 for each residue that you want to adjust. Note that no account is taken of steric clashes when selecting rotamers; however the presence of clashes is indicated by a + sign in the Clash column. If you decide that you prefer the original rotamer, you can select it in the table or click Restore to Original Conformation.

When using PrimeX, further options are available—see page 16 of the *PrimeX User Manual*.

### 5.9.3 Adjusting the Stereochemistry

The simplest way of adjusting the stereochemistry at a chiral center is to use the toolbar button,



To invert the chirality, click this button, then pick the chiral center in the Workspace. The groups to move are automatically selected, as the lowest-priority groups. You can also use this button to exchange substituents on a single atom of an aliphatic ring. To invert the chirality at all chiral centers, double-click this button. The structure is reflected in the  $xy$  plane to produce its mirror image. This procedure can be used for any structure, including fused rings.

If you want more flexibility, you can use the picking tools in the Chirality tab of the Adjust panel. You can invert the chirality of selected chiral centers or of all chiral centers. This tab also has buttons for displaying the R and S labels for the configuration at chiral centers, and for clearing the labels. If you click Label Chiral Centers, all other labels are cleared.

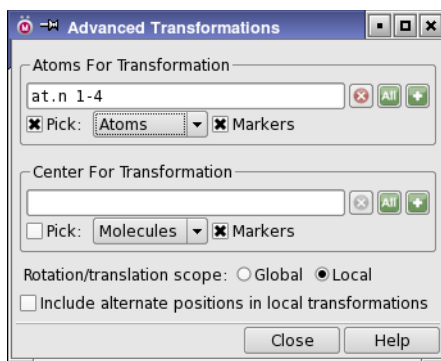
To invert the chirality at a given chiral center, select the chiral atom, then select the two other atoms that are connected to the chiral center that are to remain in place. After you have picked the third atom, the two atoms that were not picked are interchanged, with their attached groups.

You can also choose Chirality from the Adjust button menu on the Edit toolbar, and select atoms as described above.



To invert the chirality at all chiral centers, click All in the Invert chirality picking tools section.

These procedures do not apply to changing the chirality of atoms in fused ring systems at the intersection of the rings, for which the chiralities of several centers are usually related in a low-energy structure.



**Figure 5.9.** The Advanced Transformations panel.

To adjust the stereochemistry around a double bond (cis-trans isomers), choose **Convert Cis/Trans** from the **Adjust** button menu, then click on a double bond. A rotation of  $180^\circ$  around the double bond is performed, by adjusting the end that has the smallest number of attached atoms. This is the same tool as for adjusting peptide linkages, but with a different target.

### 5.9.4 Adjusting Groups of Atoms

Sometimes, you might want to adjust the position of a more general group of atoms—for example, you might want to adjust the position of a ligand with respect to a receptor, or you might want to move a functional group from one part of a molecule to another, by breaking the bonds and re-attaching it in its new location. You can do this with the local transformation tools, which are available from the **Transform** submenu of the **Edit** menu, the **Advanced Transformations** panel, and the **Transform** button menu on the **Edit** toolbar.



To open the **Advanced Transformations** panel, choose **Edit** → **Transform** → **Advanced**, or choose **Advanced** from the **Transform** button menu.

A local transformation is just like a global transformation (change of view), except that you are moving an atom subset<sup>1</sup> with respect to the other atoms in the **Workspace**. Local transformations use the same keyboard and mouse actions as global transformations.

1. The subset can in fact include all atoms in the **Workspace**, so that the rotation or translation actually changes the coordinates of the entire contents of the **Workspace**.

**To transform the selected atoms:**

1. Select the atoms in the Workspace.
2. Right-click in the Workspace and choose Transform.
3. Rotate or translate the atoms with the right or middle mouse button.

**To transform atoms by picking:**

1. Enter local transformation mode by one of the following methods:
  - Choose Edit → Transform → Pick to Transform.
  - Select Local for Rotation/translation scope in the Advanced Transformations panel.
  - Click the Transform toolbar button.
2. Choose a type of structure to pick:
  - Choose Edit → Pick → *type*.
  - Choose from the Pick menu in the Atoms for Transformation section of the Advanced Transformations panel.
  - Select the type from the Transform button menu.
3. Pick the atoms in the Workspace.

You can drag to pick multiple structural objects, but you can only pick once—you cannot add to the selection.

4. Rotate or translate the atoms with the right or middle mouse button.

Various markers are available to help in the transformation process. These markers can be turned on and off from the Transform button menu. If Show Markers is selected from this button menu, the picked atoms are marked in yellow, and the rotation center is marked in magenta. Display of the rotation center is governed by a preference—see [Section 14.4.4 on page 346](#) for details. You can also display interactions such as hydrogen bonds, contacts, and bond lengths while you are doing a local transformation. To do so, select Display Interactions or Display Bond Lengths from the Transform button menu or the Transform submenu of the Edit menu. Interactions are displayed between the moving atoms and the remaining atoms. The interactions that are displayed can be set as preferences—see [Section 14.8.2 on page 360](#) for more information.

If you want to adjust the view while you are in a transformation, hold down the SPACEBAR and change the view with the mouse buttons. This action temporarily exits local transformation mode. You can also switch modes in the Advanced Transformations panel, by selecting Global or Local under Rotation/translation scope, or by using the shortcut key CTRL+G.

More complex atom selection than a single pick can be done in the Atoms for transformation section of the Advanced Transformations panel. However, the picking tools in this section still

only allow a single pick. If you have already selected the atoms you want to transform beforehand, click the Atom Selections button and choose Workspace Selection. To select more than one group, choose Select and use the Atom Selection dialog box.



If you want to perform a rotation, a rotation center is required. By default, Maestro selects the centroid of the atoms selected for transformation as the rotation center. If this is not satisfactory, you must choose a rotation center, which you can do in the Advanced Transformations panel. You can select a new center using the tools in the Center for transformation section. Displaying atom number labels may be helpful for determining which atoms you would like to specify as the rotation center.

When you begin a local transformation, Maestro automatically begins an undo block. As a result, selecting Undo *action* from the Edit menu reverses all operations that occurred between the time that the mouse button was pressed, and the time that it was released.

If you are transforming atoms for which some or all of them have alternate positions, you can transform both alternates by selecting Include alternate positions in local transformations. To transform only the displayed set of coordinates, deselect this option. This option is also available in the Preferences panel.

### 5.9.5 Structure Sculpting

Maestro provides a special mode of local transformation called *structure sculpting*, which you enter by choosing Structure Sculpting from the Tools menu, or clicking the Sculpt button on the Build toolbar (also available from the Proteins toolbar).



In this mode, the movement of atoms is followed by a short force-field minimization that includes nearby atoms. Once you enter this mode, you can select atoms and drag them to a new location (with the left mouse button). When you release the mouse button, the minimization starts. The selected atoms are restrained. Atoms in the same residues (or molecule, if there are no residue numbers) have no constraints placed on them; atoms in complete residues that are within 5 Å of these residues are restrained, and all other atoms are frozen. The minimization proceeds for a fixed number of cycles (500) or until there is no significant change (maximum displacement of 0.005 Å). During the minimization you can continue to work on the structure. The minimization stops if you exit the mode, for example by choosing some other action that involves picking atoms, or change the content of the Workspace. If you select atoms and drag them while the minimization is proceeding, it stops and a new minimization begins.

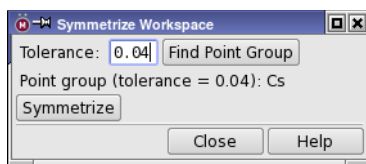


Figure 5.10. The Symmetrize Workspace panel.

## 5.9.6 Cleaning Up the Geometry

Maestro provides two tools for cleaning up the structure in the Workspace: the Geometry Symmetrizer, and the Geometry Cleanup utility. The Geometry Symmetrizer allows you to symmetrize the geometry of the structure in the Workspace, subject to a given tolerance.

### To symmetrize the Workspace structure:

1. Choose Symmetrize Workspace from the Edit menu.

The Symmetrize Workspace panel opens.

2. Click Find Point Group.

The point group found is displayed in the panel.

3. If this is not the desired point group, increase the tolerance and click Find Point Group.

4. When the desired point group is found, click Symmetrize.

Structures that are built by drawing, or have been adjusted manually, can be far from the minimum energy structure. To “clean up” the structure in the Workspace, the Geometry Cleanup utility minimizes the energy of the structure or of the selected atoms using either the built-in minimizer with the OPLS\_2005 force field, or the Universal Force Field (UFF). The choice of minimizer and force field can be set either from the Clean Up button menu or in the Preferences panel (see [Section 14.11 on page 365](#)).

Cleanup realigns atoms that are too crowded and corrects unphysical geometries. In general, it corrects distortions that can cause jobs to fail, such as MacroModel or Jaguar jobs. Minimization proceeds for 300 cycles or until the maximum atom displacement is less than 0.05 Å. By default, when using the built-in minimizer, atoms within 5 Å of the selected atoms are restrained with a moderate restraint, and atoms within 5 Å of these atoms are restrained with a much tighter restraint. The rest of the atoms are frozen, but you can set a preference to freeze all unselected atoms—see [Section 14.11 on page 365](#).

To run this utility, choose Edit → Build → Clean Up Geometry, press U, or click the Clean Up button on the Build toolbar. This job is *not* run at reduced priority, unlike most local jobs.



You can also use the built-in minimizer on the selected atoms by choosing Tools → Minimize → Selected Atoms or pressing CTRL+M (⌘M), which minimizes for 1000 cycles or a maximum displacement of 0.01 Å. If no atoms are selected, all atoms are minimized. To minimize the ligand, choose Tools → Minimize → Ligand or press CTRL+SHIFT+M (⇧⌘M).

## 5.10 Adding and Treating Hydrogen Atoms

When building molecules or preparing proteins, you might want to apply a hydrogen treatment that is compatible with the force field you intend to use in calculations on those structures. You can also use a hydrogen treatment to add hydrogen atoms to a structure that is used for any program that requires explicit hydrogen atoms, such as QikProp or Jaguar. Hydrogen treatments can treat hydrogen atoms explicitly or implicitly, as part of another atom. To select and apply a hydrogen treatment, you can use the controls in the Add Hydrogens - Advanced panel, which you open by choosing Edit → Add Hydrogens → Advanced.

To select a hydrogen treatment, choose an option from the Treatment option menu. A description of the treatment is displayed in the Description text box, including the force fields for which the treatment is valid. This information is also given in [Table 5.2](#).

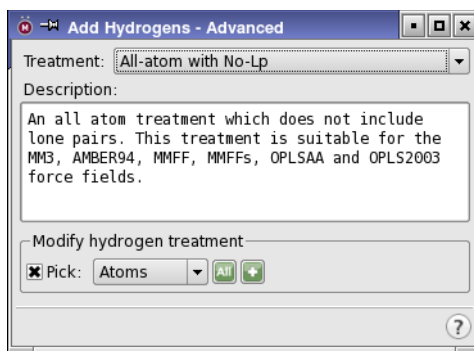
You can apply the selected treatment to the entire structure or to selected parts of the structure. To apply the treatment to the entire structure click All in the Modify Hydrogen Treatment section. To apply the treatment to selected atoms, use the picking tools in the Modify Hydrogen Treatment section or click Select to open the Atom Selection dialog box and define the selected atoms. If the structure already complies with the treatment you selected, no changes will be made when you apply the treatment.

You can also apply the current hydrogen treatment to selected atoms, molecules, residues, chains, or entries from the main toolbar or the Build panel toolbar. Select one of these structural units from the Add H button menu,



then pick atoms in the Workspace to apply the treatment. Double-click this button to apply the treatment to all atoms in the Workspace.





**Figure 5.11. The Add Hydrogens - Advanced panel.**

Each time you select a force field in the Potential section of a MacroModel or Impact energy panel, the hydrogen treatment is automatically changed to comply with that force field, and the hydrogen treatment for any atoms you subsequently draw in the Workspace will have the new hydrogen treatment. If you attempt to start a MacroModel, Impact, or Jaguar job using an input structure with an incompatible hydrogen treatment, the job fails.

*Table 5.2. Appropriate hydrogen treatments for Maestro-supported force fields.*

Hydrogen Treatment Method	MM3	MM2	AMBER	AMBER94	MMFF	MMFFS	OPLS-AA, OPLS_200x	OPLS
All-atom with No-Lp	X	X		X	X	X	X	
All-atom with Osp3-Lp		X						
Csp3 United-atom with S-Lp <sup>a</sup>			X					
Csp3 United-atom with No-Lp <sup>a</sup>								X
All atom with S-Lp			X					
Csp2/sp3 United atom with No-Lp <sup>a</sup>								X

- a. In a united atom representation, hydrogen atoms are incorporated into the dimensions of the heavy atom to which they are attached. That is, they are implicit.

## 5.11 Changing Atom Properties

In addition to changing the element and the formal charge, you can change a variety of other atom properties. The tools for making changes are in the Atom Properties tab. Each choice of property from the Property menu displays a set of tools that you can use to change the property. Apart from the Element property, the properties are listed below with a description of the tools. The last item on the menu, Other, allows you to change the values for any other atom property.

Before you change atom properties, it may be helpful to display atom labels. For atom labeling information, see [Section 8.2 on page 162](#).

### 5.11.1 Atom type (MacroModel)

When you choose Atom type (MacroModel) from the Properties menu, a list of atom type symbols with a brief description is displayed (see [Figure 5.12](#)). The atom type symbols represent atoms with specific properties, such as  $sp^3$  hybridization for a C atom with type symbol C3, or a free radical for a C atom with type symbol CR. To retype an atom, choose the atom type and click on the atoms in the Workspace that you want to change.

The use of atom types is provided primarily for MacroModel users, though Maestro always assigns an atom type to each atom. For information on atom types, see [Appendix B](#).

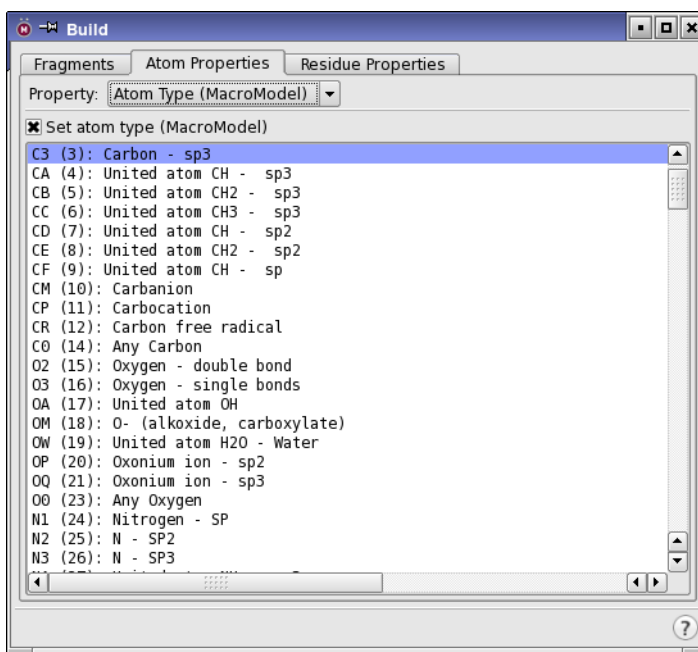


Figure 5.12. The Atom Type (MacroModel) tools in the Atom Properties tab.

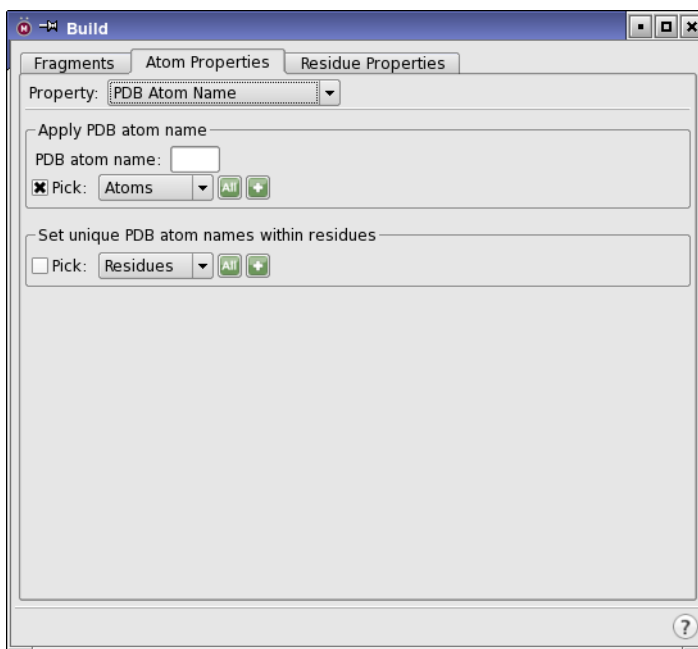


Figure 5.13. The PDB Atom Name tools in the Atom Properties tab.

### 5.11.2 Partial Charge

To apply new partial charges to atoms of interest, enter new charges in the Partial Charge and Solvation Charge text boxes, and use the picking tools to apply the partial charges to the atoms of interest. Both of these charges are used in MacroModel calculations. The solvation charge is used in MacroModel GB/SA solvation calculations. Generally, these two values should be the same. Default values for these charges are supplied with MacroModel force fields. You can also use partial charges from Jaguar electrostatic potential calculations, which are read by default when the results Jaguar calculations are incorporated or imported.

### 5.11.3 PDB Atom Name

A PDB atom name is a combination of a chemical symbol and a connection indicator. The first two characters contain the element symbol, right-justified; the third character is a remoteness indicator (A=alpha, B=beta, G=gamma, and so on), and the fourth, if it is needed, is a numeric branch designator. For instance, the name “\_CA\_” represents an alpha carbon, “\_CB\_” a beta carbon, and “\_HB\_” a hydrogen on a beta carbon. In these descriptions, the underscore characters represent spaces, which are required for compliance with PDB semantics: “CA\_\_” is a calcium atom, and is different from “\_CA\_”.

Occasionally Maestro is not able to assign PDB names to all the atoms. To manually apply missing PDB atom names, enter the desired name in the PDB atom name text box and use the Apply PDB atom name picking tools to select the atoms to which you want to apply the name.

For some purposes, such as for ligands in Prime induced fit calculations, it is useful to have unique atom names within residues. To make the atom names unique, use the Set unique PDB atom names within residues picking tools. The unique names are composed of the element symbol, right justified in the first two characters, followed by a numeric index for that element.

### 5.11.4 Atom Name

You can assign one of three types of names to atoms in the Workspace: user-specified, canonical, or unique. User-specified names can be any length. To assign a user-specified name, type the name in the Atom name text box of the Set atom name section, and use the picking tools to apply the name. You must display the atom name labels before you can see the new name.

A canonical atom name is an automatically assigned combination of atom property pairs: Element & Atom Number or Residue Number & PDB Atom Name. To assign canonical names, select the desired pair of properties from the Composition option menu, specify a separator symbol in the Separator text box, and click Apply To All Atoms. You cannot selectively apply canonical names.

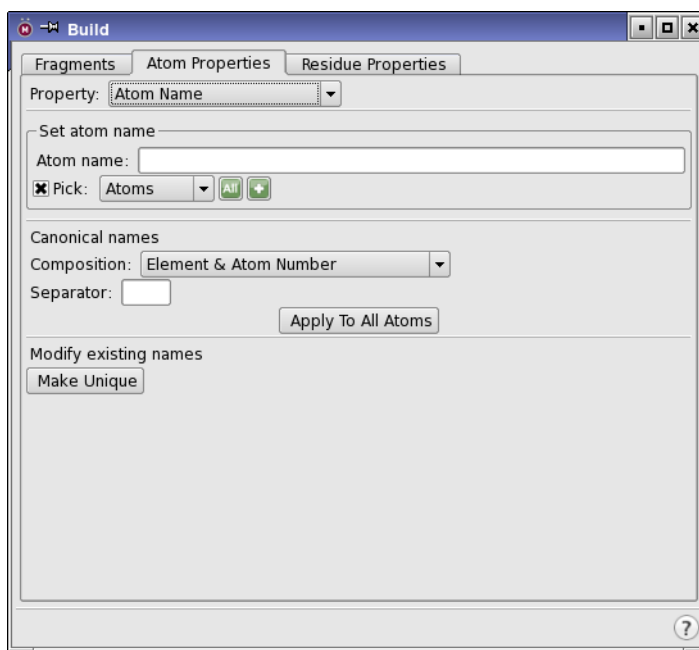


Figure 5.14. The Atom Name tools in the Atom Properties tab.

Unique names are generated using the element and atom number of each atom. If this naming scheme produces atoms with identical names, Maestro adds numeric suffixes, followed by tilde (~) symbols to distinguish the names. To apply unique names to all atoms, click Make Unique in the Modify existing names section. As for canonical names, you cannot selectively apply unique names.

### 5.11.5 Grow Name

This name is the name used internally for a fragment when growing a structure. The intended use of this property is labeling new fragments for a fragment library.

### 5.11.6 Isotope Number

To set the isotope number (mass number) for one or more atoms, choose Isotope number from the Property option menu. You can specify the isotope in the text box, then apply it to atoms with the picking tools. The isotope number is used in calculations of molecular weight.

The isotope can be displayed in an atom label in two ways. If you choose the Isotope number property to include in the atom label, it is displayed as *atom-isotope*, e.g. C-13. If you choose the mass number property, only the mass number is displayed. For hydrogen, you can set a preference to display the element label as H, D, or T, depending on the isotope number—see [Section 14.6 on page 355](#).

### 5.11.7 Other Properties

When you choose Other, the tools that are displayed allow you to change the properties for any of the properties that do not have special editing tools. These tools consist of a Properties list, which lists all the properties that have values for any of the atoms in the Workspace; an Atoms table, which lists the atoms that you choose for making changes in the properties; Add and Delete buttons, for adding and deleting properties, and Add atoms to edit their properties picking tools, for adding atoms to the Atoms table.

#### To edit one or more properties:

1. Select the desired properties in the Properties list.

The properties are added as columns to the Atoms table.

2. Use the Add atoms to edit their properties picking tools to select the atoms that you want to edit.

The atoms are listed in the Atoms table by atom number, and the property columns are populated with the values.

3. Edit the table cells to change the property values:

- To change a property for a single atom, simply edit the table cell.
- To set the value for multiple atoms, select the atom rows in the table, edit one of the table cells, and press CTRL+ENTER to apply the change to the selected rows. Selecting atoms in the table also selects them in the Workspace.

**To delete property values for all atoms in the Workspace:**

1. Choose the properties from the Property list.
2. Click Delete.

The property values are removed from all atoms in the Workspace (not just those in the table), and the property is removed from the Atoms table.

**To add a property to the atoms that are selected in the Atoms table:**

1. Click Add.

The Add Property dialog box opens.

2. Select the property type, name the property, and provide an initial value.

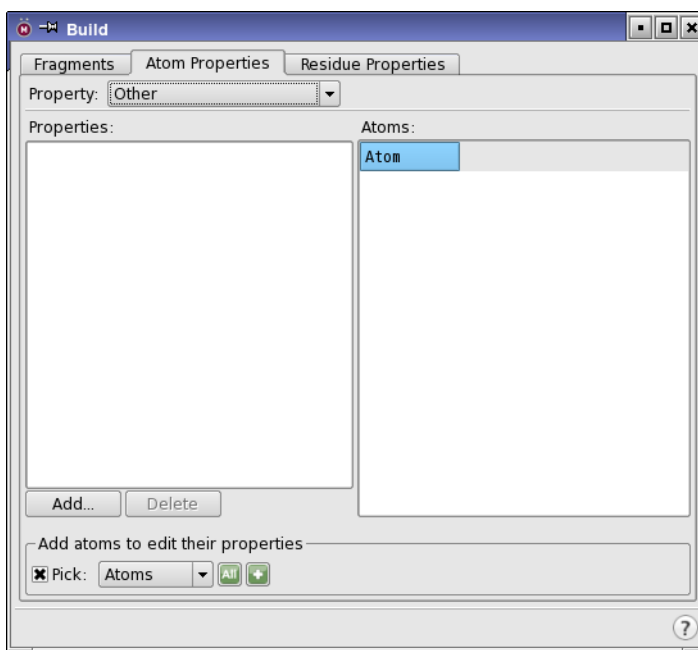


Figure 5.15. The Other tools in the Atom Properties tab.

3. Click OK.

The property is added as a column to the Property table, and the values are added to the selected atoms.

## 5.12 Changing Residue Properties

Residue properties can be changed in the Residue Properties tab. This tab is laid out in a similar fashion to the Atom Properties tab, with a Property menu and a set of tools displayed for each choice. The residue properties and their tools are described below. In order to view the results, you must first display the appropriate atom labels.

### Residue Number

To renumber more than one residue by incrementing the residue numbers, you can use the Renumber Residues section. Enter the starting value in the Renumber From text box, then use the picking tools to select the residues to renumber. The residue with the lowest number in the selection is assigned the number in the text box. The residue numbers for the remaining residues are shifted by the same amount as that of the residue with the lowest number. Renumbering therefore preserves gaps in the residue numbering. If you want to eliminate gaps, select the residues above the gap and renumber them.

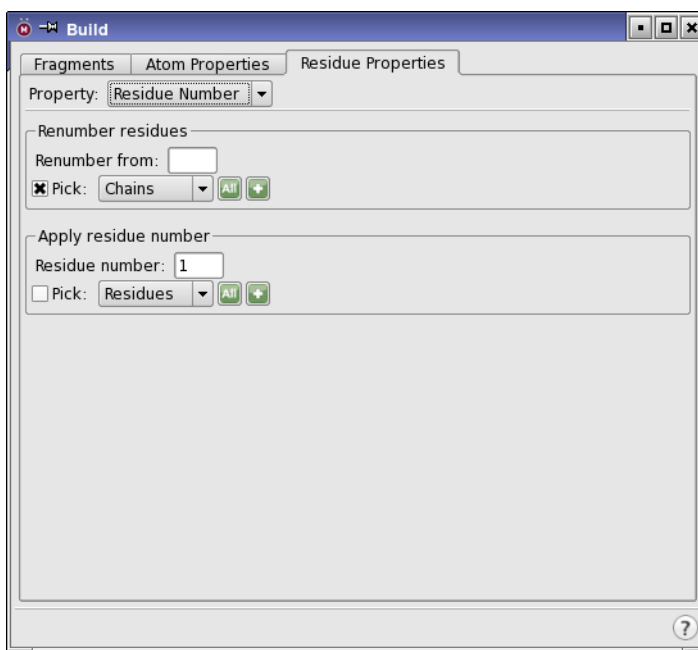


Figure 5.16. The Residue Number tools in the Residue Properties tab.

Renumbering a single residue is the same as assigning its number. To apply a specific residue number to one or more residues, in the Apply residue number section enter the number you want to apply in the Residue number text box, then use the picking tools to select the residues to apply the number to. You can also reassign the residue number of single atoms whose number is misassigned with these tools, by selecting Atoms from the Pick option menu, then picking the atom to assign the specified residue number.

### Residue Name

To name residues, enter the residue PDB name in the Residue PDB name text box, and use the picking tools to select the residues to name. PDB residue names are three characters long and are right-justified. For example, the residue name G3 must be entered with a leading space, as “ G3”, whereas the residue name C19 should have no leading space, “C19”.

### Chain Name

You can assign a single-letter name to chains. The definition of a chain is not restricted to the items labeled Chain in the pick option menus: you can define a chain in any way that you like, and assign it a name. To assign the name, enter a character in the Chain Name text box and use the picking tools to select the chain. To remove a chain name, clear the Chain Name text box and use the picking tools to select the chain.

## 5.13 Defining Dummy Atoms

Dummy atoms are used by several of the computational programs for defining geometries and geometric parameters. You can retype an atom to a dummy atom type using the MacroModel Types atom property described earlier. You can also place a dummy atom at the centroid (mean position) of a group of atoms, such as a ring. You can then change the dummy atom to a real atom, and thus place real atoms at the centroid of some system of interest.

The centroid capability is available in the Centroids panel, which you open from the Edit menu, and is docked into the Workspace by default. To define a centroid, use the picking tools in the Define atoms for centroid section. The atoms are listed in the Atoms to define centroid list. If you have Markers selected, the atoms are marked with a salmon-colored star, and the atom that is selected in the list is marked with a lavender-colored star. You can delete atoms from the list by selecting the list item and clicking Delete. Once you have picked all the atoms, click Create Centroid Atom. To define another centroid, click Delete All before picking atoms for the new centroid.



## 5.14 Deleting Atoms and Bonds

If you need to delete atoms from a structure, you can use the Delete submenu of the Edit menu or the Delete button menu on the Edit toolbar or the Build toolbar.



These menus offer choices for the type of object to delete, and allow you to open the Atom Selection dialog box to select atoms for deletion based on their properties. You can also select atoms in the Workspace, then click the Delete button, press DEL, or use the shortcut menu to delete them.

When you delete atoms, the terminal atoms that are attached to this atom can be deleted, or the terminal atoms can be left in place. Terminal atoms are atoms that are bonded only to that atom, such as hydrogen or a halogen. Deleting terminal atoms would not, for example, delete a methyl group attached to the deleted atom. This action is controlled by an option that you can set in the Builder tab of the Preferences panel.

Another means of deleting atoms is to select them and choose Edit → Cut or press CTRL+X. The atoms are removed from the structure and placed on the clipboard. You can then paste these atoms into the Workspace later, as a scratch entry.

If you want to remove all atoms in the Workspace, choose Workspace → Clear or use the Clear Workspace button, which is located on the main toolbar. This action does not delete the atoms from the structure, it only removes them from the Workspace.

If you want to delete bonds, either to create new ones or to split a molecule into smaller pieces, you can, you can right-click and hold on a bond in the Workspace and choose Delete from the

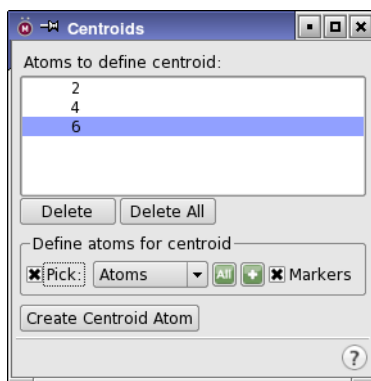


Figure 5.17. The Centroids panel.

shortcut menu, or choose Bonds from the Delete button menu on the Edit toolbar or the Build toolbar, then click on the bond to delete.



Zero-order bonds are a special type of bond that are used to define connectivity when a fragment “belongs” to a molecule. Two fragments that are joined by a zero-order bond are considered to be a single molecule in Maestro. One instance where zero-order bonds are used is for a metal atom in a complex, where for purposes of force-field calculations it must be treated as an ion, but for purposes of connectivity it is considered part of the complex. You can delete zero-order bonds in the same way as regular bonds, and you can delete all zero-order bonds by choosing Zero Order Bonds from the Delete button menu.

# Selecting Atoms

Maestro has a powerful set of tools for selecting atoms in a structure: toolbar buttons, picking tools in panels, and the Atom Selection dialog box. These tools allow you to select atoms in two ways:

- Select atoms first and apply an action to them
- Choose an action first and then select atoms for that action

## 6.1 Picking in the Workspace

One of the primary means of selecting atoms is to pick atoms in the Workspace. The tools with which you can do so are described in later sections. To pick an atom, you click on the atom. The atom is then selected. If you want to select multiple atoms, you can drag over the region containing those atoms, and they are all selected. If you want to add atoms to the selection, hold down **SHIFT** while you click or drag. To invert the selection of atoms (select the unselected atoms, deselect the selected atoms), hold down **CTRL** while you click or drag. If you click or drag in an empty part of the Workspace, the selection is cleared. Dragging over ribbons when the associated atoms are not displayed selects the associated atoms inside the rectangle.

The Selection shortcut menu also has some items for selecting atoms. You can invert the selection, and you can extend the selection to atoms within a radius or atoms that match by color, representation, or element. See [Table 2.3 on page 29](#) for information on this shortcut menu.

## 6.2 Using the Toolbar Buttons

The small triangle in the lower right corner of a toolbar button indicates that the button contains a menu. Many of these buttons allow you to choose a structural unit for selecting. Choose **Atoms**, **Bonds**, **Residues**, **Chains**, **Molecules**, or **Entries**, then click on an atom in the Workspace to perform the action on all the atoms in that structural unit.

For example, to select atoms in residues with the **Select** button:

1. Choose **Residues** from the **Select** button menu:



The button changes to:



2. Click on an atom in a residue in the Workspace to select all the atoms in that residue.

The Select button is the primary means of selecting atoms in the Workspace prior to performing an action.

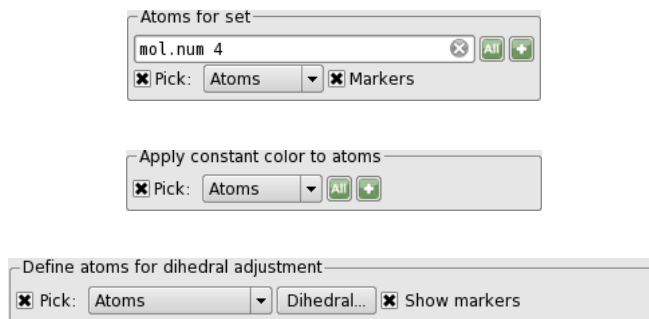
In addition to selecting atoms by picking, you can expand the selection to include atoms within a given distance of the current selection. To include all atoms in residues that have any atoms within the specified distance, select **Expand Residues** on the Select button menu. If this option is not selected, only the atoms within the specified distance are added. To expand the selection, choose the distance from the Select button menu, or choose **Custom** and enter the distance in the dialog box that opens.

If you want to replace the selection with the atoms within a given distance of the selection, select **Exclude Selected** from the Select atoms button menu. This is useful if, for example, the ligand is selected, and you want to select the receptor residues that are within a given distance of the ligand, but not include the ligand in the selection.

These tools are also available from the **Expand Selection** submenu of the Selection shortcut menu (see [Section 2.7](#) on page 27).

If you want to select all atoms in a particular category, you can choose the category from the Select button menu. The available categories are:

- **All**—all atoms in the Workspace.
- **Displayed Atoms**—atoms that are displayed in the Workspace.
- **Protein**—protein atoms (backbone and side chain).
- **Protein Backbone**—protein backbone atoms.
- **Protein Side Chains**—protein side chain atoms.
- **Protein Near Ligand**—protein residues within 5 Å of the ligand.
- **Ligands**—ligand atoms, as defined in the Ligand Detection Settings dialog box.
- **Waters**—all water molecule atoms.
- **Ions**—charged atoms and molecules that have less than 10 atoms.
- **Metals**—all elements to the left of B, Si, Ge, Sb, Po in the periodic table.
- **Heavy Atoms**—all non-hydrogen atoms.
- **All Hydrogens**—all hydrogen atoms.
- **Nonpolar Hydrogens**—hydrogen atoms bonded to carbon.
- **Nonpolar Ligand Hydrogens**—hydrogen atoms bonded to ligand carbon atoms.
- **Polar Hydrogens**—hydrogen atoms bonded to atoms other than carbon.
- **Membrane**—atoms in membrane molecules (POP, POPC, POPE, DPPC, DPMC).



**Figure 6.1.** Examples of picking tools. Top: from the Sets panel; Center: from the Atom and Bond Coloring panel; Bottom: from the Adjust panel.

These categories are available on other toolbar buttons that allow you to pick atoms.

## 6.3 Using the Picking Tools

The picking tools are embedded in each panel in which you need to select atoms to apply an operation. The picking tools in a panel can include one or more of the following:

- Pick option menu—Allows you to choose a structural unit for selecting atoms. The pick option menu is described on [page 123](#).
- Dihedral button—Opens the Dihedral Selection dialog box, in which you can select protein dihedral angles.
- Markers option—Marks the selected atoms in the Workspace
- Text box—Allows you to type in an ASL expression, and displays the ASL expression for the current selection. ASL stands for Atom Specification Language, and is described in detail in the *Maestro Command Reference Manual*.
- Clear button—Clears the current selection. This button is displayed in the text box when an expression is present.



- All button—Selects all atoms in the Workspace. This includes atoms that are not displayed.



- Atom Selections button—This button displays a list of common atom categories that can be selected when you click it. Clicking one of the items acts on the corresponding atoms, if the action is immediate, or adds the atoms to the selection, if the action is performed later. It also has two buttons, to build or recall atom selections using ASL expressions.



The atom categories that you can act on or add to the selection are:

- Workspace Selection—atoms that are already selected in the Workspace.
- Displayed Atoms—atoms that are displayed in the Workspace.
- Protein—protein atoms (backbone and side chain).
- Protein Backbone—protein backbone atoms.
- Protein Side Chains—protein side chain atoms.
- Protein Near Ligand—protein residues within 5 Å of the ligand.
- Ligands—ligand atoms, as defined in the Ligand Detection Settings dialog box.
- Waters— all water molecule atoms.
- Ions— charged atoms and molecules that have less than 10 atoms.
- Metals—all elements to the left of B, Si, Ge, Sb, Po in the periodic table.
- Heavy Atoms—all non-hydrogen atoms.
- Hydrogens-All—all hydrogen atoms.
- Hydrogens-Nonpolar— hydrogen atoms bonded to carbon.
- Hydrogens-Nonpolar Ligand— hydrogen atoms bonded to ligand carbon atoms.
- Hydrogens-Polar— hydrogen atoms bonded to atoms other than carbon.
- Membrane—atoms in membrane molecules (POP, POPC, POPE, DPPC, DPMC).

These are the same as on the Select button menu (and other button menus), except for the first item.

The two buttons are:

- Select—Opens the Atom Selection dialog box (see [Section 6.5 on page 125](#))
- Previous—Performs the action on the most recent atom selection defined in the Atom Selection dialog box (see [Section 6.5 on page 125](#)).

The range of picking tools available in a panel varies according to the types of structural units that are needed for the operation and whether picking causes immediate action or requires an action to be specified later. The ASL text box and Clear button are included only when picking merely defines a set of atoms for later use. For example, the Dihedral tab of the Adjust panel has a Pick option menu and a Dihedral button, and the action is immediate. The Sets panel has a full set of picking tools, and stores the atoms in a defined set that can be used later. When picking for an action to be performed later, each picking action adds atoms to the ASL expression (with an implicit OR), which is (with an implicit OR) shown in the ASL text box.

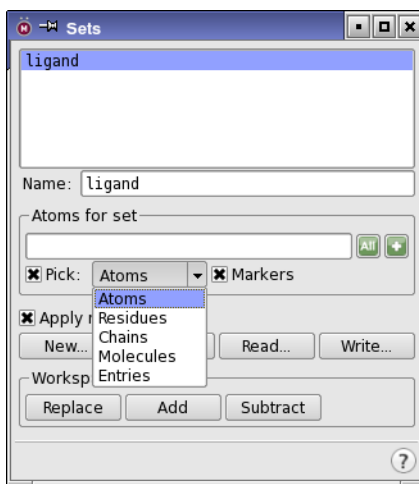


Figure 6.3. The Sets panel, showing the Pick option menu.

### 6.3.1 The Pick Option Menu

With the Pick option menu, you can choose a structural unit (Atoms, Bonds, Residues, Chains, Molecules, or Entries) and click on an atom or a bond in the Workspace to select all the atoms in that structural unit. For instance, choose Atoms and click on an atom in the Workspace to select just that atom. Choose Residues and click on an atom to select all the atoms in that residue. Choose Bonds and click on a bond to select both atoms that define that bond.

When you select a structural unit, the cursor in the Workspace appears as a box with a letter: A, B, R, C, M, and E represent Atoms, Bonds, Residues, Chains, Molecules, and Entries, respectively. Successive clicks add atoms to the selection.

If you want to know the index of structural unit that you are picking (for example, the molecule number), you can set a preference to show the index in the status bar. When the pointer is over an atom, the index of the structural unit is displayed as Pick: *index* at the beginning of the status bar. See [Section 14.5.1 on page 354](#) for details on the preference.

The number of structural units available in the menu depends on the operation. For instance, when you define a dihedral angle, you can pick either four atoms or three bonds. The Pick option menu for this operation therefore only contains Atoms and Bonds.

You do not need to select the Pick option before choosing an item from the Pick option menu; it is automatically selected when you choose a menu item.

### 6.3.2 The Dihedral Selection Dialog Box

For proteins, you can select the dihedrals by name in the Dihedral Selection dialog box, which you open by clicking the Dihedral button in the picking tools.

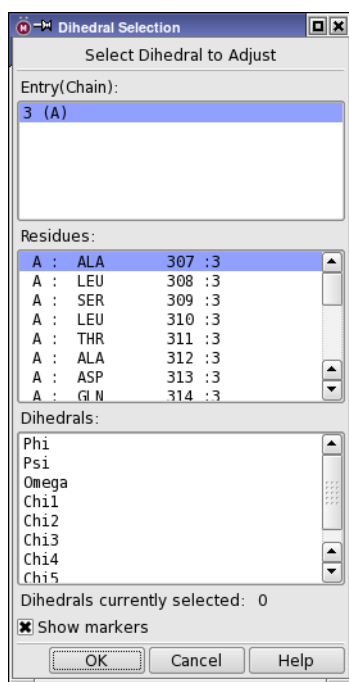
**To select one or more dihedral angles:**

1. Select one or more chains in the Entry (Chain) list.

The list of residues in the selected chains is displayed in the Residues list.

2. Select one or more residues in the Residues list.
3. Select the dihedrals in the Dihedrals list.

The dihedrals are selected for each selected residue, and the number of dihedrals is displayed below the table. If Show markers is selected, the dihedrals are marked in the Workspace.



**Figure 6.4.** The Dihedral Selection dialog box.



## 6.4 Using the Edit Menu

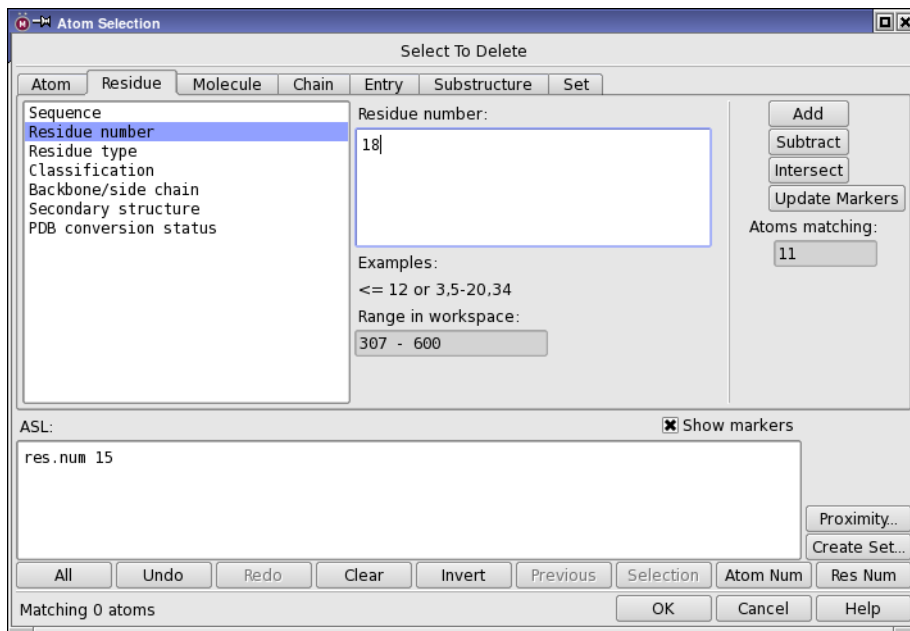
The Edit menu also has a set of tools for picking atoms, on the Pick and Select Atoms submenus. You can choose the structural unit to pick from the Pick submenu, which also sets the structural unit on the Select atoms toolbar button menu. To pick atoms, choose Edit → Select Atoms → Pick to Select, which is the same as clicking the Select atoms toolbar button, or pressing the ` key (backquote).

In addition to selecting atoms by picking, the Select Atoms submenu has items to invert the selection, select the previous or next residue, or open the Atom Selection dialog box.

## 6.5 The Atom Selection Dialog Box

If you want to make atom selections based on more complex criteria, such as selecting all the carbon atoms in a protein backbone, you can use the Atom Selection dialog box. The Atom Selection dialog box allows you to select atoms by defining complicated ASL expressions without the need to understand the ASL syntax.

To open the Atom Selection dialog box, choose Select from a button menu or click Select in the picking tools of a panel. The Atom Selection dialog box is modal: you must dismiss it before



**Figure 6.5.** The Atom Selection dialog box.

you can perform any other operations, with the exception of rotation and translation of structures and selecting atoms in the Workspace.

When you close the Atom Selection dialog box, the ASL expression is automatically stored and can be recalled with the Previous button on any set of picking tools.

### To select atoms

1. Create an atom group by selecting a property and value (see [Section 6.5.1 on page 126](#)).
2. Click Add or Subtract to define the current selection (see [Section 6.5.4 on page 127](#)).
3. Create more atom groups as needed and click Add, Subtract, or Intersect to modify the current selection (see [Section 6.5.4 on page 127](#)).
4. When you are satisfied with the current selection, click OK to apply the operation to the selection.

Some operations, such as deleting atoms, take effect immediately. Others merely define a set of atoms to be used in a subsequent task, such as selecting atoms for creation of a surface.

The features of the Atom Selection dialog box are described in the following sections.

### 6.5.1 Selecting Atoms by Property

You can create an atom group by selecting a property and a value for that property. These properties are grouped into a number of categories, each in their own tab: Atom, Residue, Molecule, Chain, and Entry. For each category there is a list of properties shown on the left of the tab, from which you can select one item. When you select an item, tools for that property are displayed in the center of the tab. The three types of tools are:

- Text box. You can specify the allowed values for the property by using lists of numbers, closed ranges (e.g. 12-42) and open ranges (e.g.  $\geq 30$ ).
- List. You can choose one or more entries from the list by clicking, in combination with the SHIFT and CTRL keys. Only items that are currently in the Workspace are displayed in the list.
- Set of options, which can be nested. You can choose only one of the possible combinations by selecting the options.

With text boxes and lists, you can also choose items by selecting atoms in the Workspace. For example, if you choose the Element property in the Atom category, then select a carbon atom in the Workspace, the “C” item in the list of elements is selected.

The current atom group is represented in two ways: the atoms are marked in purple in the Workspace (if Show markers is selected) and the value in the Atoms Matching field indicates how many atoms are matched by the current property specification.

### 6.5.2 Selecting Atoms by Connectivity

You can create an atom group by specifying a substructure in the Substructure tab that defines the connectivity of the atoms. This is a convenient way of selecting all instances of a particular functional group, for example.

Maestro provides access to two substructure notations, SMARTS, and Maestro. The Maestro substructure notation is described in [Appendix C](#), and is similar to SMARTS. To select atoms that match a particular substructure, type the pattern for the substructure in the text area. If you select SMARTS notation, you can automatically generate the pattern from the Workspace selection by clicking Get From Selection. You can make the selection in the Workspace while the Atom Selection dialog box is open. A SMARTS pattern that matches the selection replaces the content of the text area. If there are many atoms in the Workspace, it may take some time. You can set preferences for some of the notational elements in the SMARTS pattern—see [Section 14.14 on page 375](#).

### 6.5.3 Selecting Atoms Using Previously Defined Sets or Selections

In the Sets tab, you can select atom sets that have been defined previously. Maestro provides a list of predefined atom sets. You can also define your own sets, either directly in the Sets panel, or by using the Atom Selection dialog box to select the atoms, then clicking Create Set. These named sets are stored with the project and are available in the Sets tab. The sets are stored as ASL expressions, unless you convert them to a list of atom or residue numbers. They can therefore be transferred from one structure to another. You can use the Sets panel to select atoms in any of the sets you have created—see [Section 10.4 on page 256](#) for details.

There are two other ways of recalling a previously defined atom selection. The first is to click Previous (below the ASL text box), which recalls the atom selection defined the last time the Atom Selection dialog box was used. The second is to click Selection, which uses the atoms that are selected in the Workspace as the ASL expression. Both of these buttons replace the current ASL expression: any existing expression is lost. You can add to these expressions, so they are useful as a starting point for a more complex expression.

### 6.5.4 Combining and Modifying Atom Selections

Once you have created an atom group, you can combine it with the current selection. The Add, Subtract, and Intersect buttons combine the ASL expression for the atom group with the existing ASL expression in the ASL text box (the current selection), as follows:

- The Add button includes the atom group in the current selection by performing a boolean OR operation on the ASL expressions.
- The Subtract button excludes the atom group from the current selection by performing a boolean AND NOT operation on the ASL expressions.
- The Intersect button restricts the selection to the atoms that are in both the atom group and the current selection by performing a boolean AND operation on the ASL expressions.

**Note:** Intersect is not available for the first atom group that is defined.

In addition to combining ASL expressions to modify the current selection, you can use the following buttons:

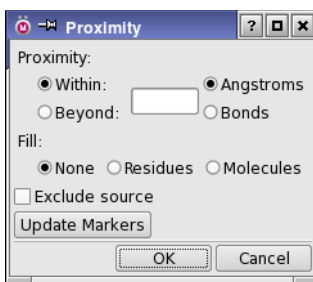
- All—select all atoms in the Workspace. Replaces the existing expression.
- Undo—undo the last operation
- Redo—redo the last operation
- Clear—clear the ASL expression
- Invert—negate an entire expression
- Previous—recall the atom selection defined the last time the Atom Selection dialog box was used. Replaces the existing expression.
- Selection—use the atoms that are selected in the Workspace as the ASL expression. Replaces the existing expression.
- Atom Num—convert the ASL expression to list each atom explicitly by atom number
- Res Num—convert the ASL expression to list each residue explicitly by residue number

If Show Markers is selected, the atoms corresponding to the current selection (the expression in the ASL text box) are highlighted with light blue markers in the Workspace.

### 6.5.5 Selecting Atoms by Proximity

Once you have made an initial selection, you can select atoms based on their distance from the atoms defined by the current ASL expression (the source atoms) in the Proximity dialog box, see [Figure 6.6 on page 129](#). To open this dialog box, click Proximity.

You can specify the distance in angstroms or in terms of the number of bonds. If the boundary for inclusion intersects a molecule or a residue, you can choose to include the entire molecule or residue using the Fill buttons.



**Figure 6.6.** The Proximity dialog box.

You can either include or exclude the source atoms in the selection. For example, you might want to include residues within a certain distance of a metal atom, but not include the atom itself. The Update Markers button updates the markers for the proximity selection so that you can view the selection in the workspace before accepting it.

### 6.5.6 Editing and Storing Expressions

You can undo multiple operations with repeated clicks on the Undo button. The Redo button reverses undo operations, and can also be used multiple times. (These are the buttons in the dialog box, not the toolbar button.)

You can also type ASL expressions directly into the ASL text box. The hand-edited expressions are considered part of the last operation performed with the mouse and can be undone and redone as part of that operation, but cannot be undone or redone separately.

The Create Set button opens a dialog box that enables you to name and store the existing ASL expression for use as a set definition. The sets created in this manner are the same as sets created with the Sets panel, and are listed in the Set tab. You can therefore create sets from the Atom Selection dialog box, and use them for atom selection later. For more information on creating and saving sets, see [Section 10.4 on page 256](#).

### 6.5.7 Converting Expressions to Lists

ASL expressions are stored as formal expressions that can be applied in different contexts to select different sets of atoms. If you want an expression that explicitly lists the atom numbers or the residue numbers, you can convert the ASL expression in the ASL text box into a list of atoms by clicking Atom Num, or into a list of residues by clicking Res Num.

## 6.5.8 Examples of Atom Selection

Below are some examples of the use of the Atom Selection dialog box. It is assumed that you have the Atom Selection dialog box open. To apply your selection and dismiss the dialog box, click OK. These examples assume that the protein and the ligand are in separate entries in the Workspace.

### To select all carbon atoms in the backbone of a protein:

1. In the Atom tab, select Element from the list of properties.
2. Select C from the list of elements.
3. Click Add to add the atom group to the ASL expression.
4. Select Backbone/Side Chain from the list of properties.
5. Select the Backbone option.
6. Click Intersect to restrict the current ASL expression to be applied only to protein backbone atoms.

If you want to continue to the next example, click Clear to clear the current ASL expression.

### To select all side chains within 5.0 Å of a ligand in the active site of a ligand/receptor complex:

1. In the Entry tab, select the entry name for the ligand from the list of entries.
2. Click Add to make this entry name the current ASL expression.
3. Click Proximity to open the Proximity dialog box
4. Enter 5.0 in the text box, click Residues in the Fill section, select Exclude source, then click OK.
5. In the Residue tab, select the Backbone/Side Chain property.
6. Select the Sidechain option.
7. Click Intersect to restrict the current ASL expression to include only atoms in the protein side chain.
8. If you want to continue to the next example, click Clear to clear the current ASL expression.

**To select a range of residues but exclude proline residues:**

1. In the Residue tab, select Sequence from the property list.
2. Select the appropriate chain from the list of chains in the top scrolling list.
3. Select a range of residues in that chain from the lower scrolling list.
4. Click Add to make this residue range the current ASL expression.
5. Select the Residue Type property.
6. Select PRO from the list of residue types.
7. Click Subtract to exclude proline residues from the current ASL expression.

## 6.6 Storing the Workspace Selection

When you have made an atom selection, you can also store the selection in a memory location. To do so, ensure that the pointer is in the Workspace, then press CTRL+*numeral-key* (for example, CTRL+3), or choose Edit → Select Atoms → Save → Selection *number*. The selection is stored in the memory location corresponding to the numeral key or number. To retrieve the selection, simply press the numeral key when the pointer is in the Workspace, or choose Edit → Select Atoms → Restore → Atom Selection *number*.

Selections are stored as an ASL expression that consists of the atom numbers relative to the Workspace of the selected atoms. When you change the contents of the Workspace, the atom numbers can change. If you retrieve a selection from memory after changing the Workspace contents, the selection is applied to the current atom numbering, and might result in a selection that is different from what you expected. However, if you replace the Workspace contents with a conformer of the previous contents, for example, the stored atom selections should apply to the corresponding atoms in the conformer.

For a more general storage facility, you can create atom sets in the Sets panel. See [Section 10.4 on page 256](#) for more information. These stored selections are not the same as the named atom sets, as they can only be defined and used in the Workspace.





# Changing the Appearance of Structures

Maestro provides a wide selection of options for displaying structures. For example, you can change the color of some or all of the atoms, change the molecular representation in which the atoms are depicted, label atoms by their properties, or selectively undisplay certain atoms so that you can better examine small subsections of a structure.

## 7.1 The Representation Toolbar

Many of the features for changing the appearance of structures are available from the Representation toolbar. The toolbar buttons are described in brief below, and their use is discussed in the following sections.



### Ribbon

Show, hide, or color ribbons. From the button menu you can choose to display ribbons for all, selected, or displayed residues; delete ribbons; and display various combinations of atoms that are associated with the ribbons; and choose various coloring schemes for the ribbons. Click to pick residues for display of ribbons. Double-click to display ribbons for the selected atoms, or for all atoms if no atoms are selected.



### Wire

Draw bonds in wire frame representation. From the button menu you can select a structural unit to use when picking atoms to display in wire representation. Double-click to apply to the selected bonds, or to all bonds if there is no selection.



### CPK

Draw atoms in CPK representation. From the button menu you can select a structural unit to use when picking atoms to display in CPK representation. Double-click to apply to the selected atoms, or to all atoms if there is no selection.



### Ball & Stick

Draw atoms and bonds in ball-and-stick representation. From the button menu you can select a structural unit to use when picking atoms to display in Ball & Stick representation. Double-click to apply to the selected atoms, or to all atoms if there is no selection.



### Tube

Draw bonds in tube representation. From the button menu you can select a structural unit to use when picking atoms to display in tube representation. Double-click to apply to the selected bonds, or to all bonds if there is no selection.



### Thin Tube

Draw bonds in thin tube representation. From the button menu you can select a structural unit to use when picking atoms to display in tube representation. Double-click to apply to the selected bonds, or to all bonds if there is no selection.



### Color Scheme

Color all atoms with a chosen color scheme. From the button menu you can choose the scheme, as defined in the Color Schemes tab of the Atom Coloring panel. The custom color schemes for carbon atoms and ligands are on a submenu.



### Color

Color the picked residues with a constant color, which you can choose from the button menu. Double-click to apply the color to the selected atoms, or to all atoms if there is no selection.

## 7.2 Changing Atom, Bond, and Background Color

Changing the color of a structure can help you to visualize its properties and its three dimensional structure. The Atom and Bond Coloring panel allows you to apply a new color to all or some of the Workspace atoms and bonds, or to use predefined or user-defined schemes to color specific atom groups. You can also use the shortcuts available in the toolbar to change the atom coloring. The default color is set in the Preferences panel—see [Section 14.13.1 on page 371](#).

To open the Atom and Bond Coloring panel, choose Workspace → Atom and Bond Coloring.

This panel is a dockable panel, that opens by default docked in the main window. To change this behavior you can set preferences—see [Section 14.1.6 on page 335](#).

### 7.2.1 Applying a Single Color to Atoms and Bonds

To apply a single color to some or all atoms or bonds in the Workspace, you can use the tools in the Atom Color or Bond Color tab. Select Constant color under Color atoms by or Color bonds by, then select a color by clicking the color button in the Atom Color tab to open a standard color selector, or clicking the color button in the Bond Color tab to display a color palette. Once you have selected a color, use the picking tools or the selection button in the Apply constant color section to apply the color to selected atoms or bonds. For a wider range of bond colors,

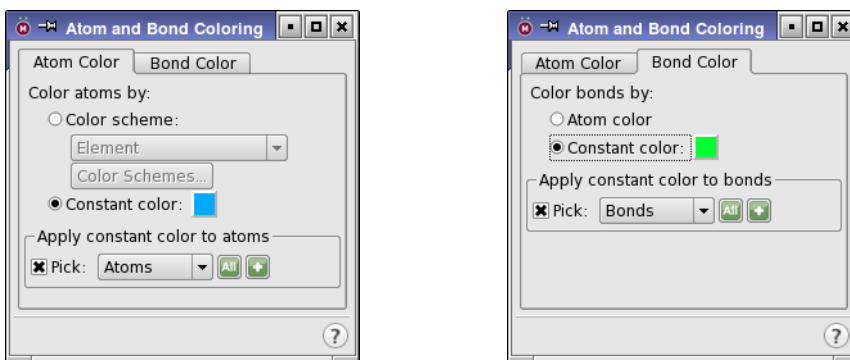


Figure 7.1. The Atom and Bond Coloring panel, showing both tabs.

the color palette has an Advanced button, which opens the Choose Color dialog box, where you can modify the palette and choose colors by RGB value.

You can also apply a color from the Color button menu on the Representation toolbar.



This button displays a menu from which you can choose from a selection of colors. The color choice is persistent. You can then pick residues to apply the color, or double-click the button to apply the color to all atoms. If the color you want to use is not on the menu, you can use the Atom Color tab to select the color. The RGB value of the colors in the color palette is displayed in a tool tip. For information on customizing the colors, see [Section 13.5.2 on page 321](#).

### 7.2.2 Coloring Bonds by Atom Colors

If you want half-bonds to be colored by the atom color, select Atom color under Color bonds by in the Bond Color tab. This option ties the bond color to the atom color, regardless of how the atom is colored.

### 7.2.3 Using Color Schemes to Color Atoms

To apply coloring to some or all Workspace atoms using one of Maestro's predefined color schemes, or a custom color scheme, select Color Scheme under Color atoms by in the Atom Color tab, then select the scheme from the option menu below this option. If you choose one of the schemes with custom colors (for carbons or ligands), choose the color from the custom color option menu (labeled Carbon color or Ligand color). Once you have selected a scheme, use the picking tools to select the atoms you wish to color.

You can apply a color scheme to all atoms in the Workspace from the Color all atoms by scheme button menu in the toolbar.



When you click and hold on this icon a menu is displayed from which you can choose the scheme. The custom carbon and custom ligand schemes are in submenus. The color scheme is applied when you make your menu choice.

If you want to see a description of the color scheme, click Color Schemes, which opens the Color Schemes panel. This panel allows you to view the description of the color scheme. For details of the actual colors applied, click Edit in this panel. The Edit Color Schemes dialog box lists the details of the colors and the criteria used to apply them. Use of this panel is described below. The standard color schemes are described in [Table 7.1](#).

Table 7.1. Standard color schemes

Scheme	Description
Atom PDB B Factor (Temperature Factor)	Apply a spectrum of colors to atoms depending on the PDB temperature factor (B factor).
Atom Partial Charge	Apply a spectrum of colors to denote sign and magnitude of charge.
Atom Type (MacroModel)	Colors each atom type by the older MacroModel coloring scheme.
Chain Name	Color each chain with a unique color corresponding to its single-letter name.
Density Fit	Color atoms according to the value of the PrimeX density fit.
Element	Color atoms according to their atomic number. Light elements continue to have their standard Maestro colors, as in the Atom Type scheme. Other elements are divided into several groups, and each group has a unique color. For example, the first row of transition metals is turquoise. In this color scheme, atoms of the same element are always the same color, regardless of their formal charge or MacroModel atom type. This is the default coloring scheme.
Element (Light Carbons)	Color atoms according to their atomic number, as in the Element scheme, except that carbon atoms are light gray, and hydrogens are cyan.
Element ( <i>color</i> Carbons)	Color atoms according to their atomic number, as in the Element scheme, except that carbon atoms are colored with the stated color. These schemes appear under the heading Element (Custom Carbons).
Element ( <i>color</i> Ligand)	Color atoms according to their atomic number, as in the Element scheme, except that atoms in the ligand are colored with the stated color. These schemes appear under the heading Element (Custom Ligand).
Element (Entry Carbons)	Color all atoms except carbon atoms according to their atomic number, as in the Element scheme, and colors carbon atoms by entry number, cycling through a list of 12 colors.
Element (Chain Name Carbons)	Colors carbon atoms by chain name, using 26 colors for names A–Z and repeating for names 1–26, and colors other atoms by Element.
Element (Molecule Number Carbons)	Colors carbon atoms by molecule number, cycling through a list of 12 colors, and colors other atoms by Element.
Entry	Colors atoms according to the entry to which they belong. The scheme cycles through a list of 12 colors.
Entry ID	Colors atoms according to the entry ID of the entry to which they belong. The scheme uses a list of 12 colors, applying them by the value of the entry ID, modulo 12: thus, each entry whose remainder when the entry ID is divided by 12 has the same color.

Table 7.1. Standard color schemes (Continued)

Scheme	Description
Hydrophobicity	Three schemes for hydrophobicity are available: Li-Tang-Wingreen (Phys. Rev. Lett. 1997, 79, 765), Kyte-Doolittle (J. Mol. Biol 1982 157, 105), and Black-Mould (Anal. Biochem. 1991, 193, 72). All three schemes rely on the residue name to determine the appropriate property value for the color scheme.
Molecule Number	Color each molecule by number. The scheme cycles through a list of 12 colors.
Molecule Size	Color atoms by molecule size, making it easier to locate ligands in a structure.
PDB Conversion Status	Color residues in structures imported from the PDB by the status of their conversion: Gray Standard residues, no conversion problems Green Residue with alternate position indicator Blue Standard residue with unknown atom names Cyan Residue adjacent to gap Red Standard residue with missing atoms Orange Non-standard residue, bond orders may need correcting
Residue Charge	Color amino acid residues according to charge. Positive charges are blue, negative charges are red.
Residue Property	Color amino acid residues according to hydrophobicity, charge, and polarity. gray GLY and atoms without PDB residue names dark green Hydrophobic residues: ALA, CYS, ILE, LEU, MET, PHE, TRP, TYR, VAL, PRO cyan Polar uncharged: SER, THR, HIS, GLN, ASN blue Positively charged: LYS, ARG red Negatively charged ASP, GLU purple Purines: G, A, I sienna Pyrimidines: C, T, U
Residue Position	Color amino acid residues by residue number. The first 10% (including the N-terminus) of the residues in a chain are dark blue, the last 10% (C-terminus) are red and there is a color ramp between those ends.
Residue Type	Color amino acid residues by residue type.
Residue Type (spectrum)	Color amino acid residues by residue type, with finer distinctions between conservatively mutated and conserved residues.
Secondary Structure	Color residues according to protein secondary structure (strand, loop, helix). To assign secondary structure, choose Assign Secondary Structure from the Tools menu.

## 7.2.4 Creating and Editing Color Schemes

If you want to adjust an existing color scheme, or create a new color scheme, click Color Scheme in the Atom Color tab of the Atom and Bond Coloring panel. The Color Schemes panel opens, in which you can edit an existing color scheme, copy an existing scheme to edit, or create a new scheme from an atom property.

To examine or edit a color scheme, first select it in the color schemes list. The list is synchronized with the Color scheme option menu in the Atom Color tab of the Atom and Bond Coloring panel, so the scheme you chose in that panel is the default selection in the color scheme list.

New color schemes can be created from atom properties for which schemes do not already exist. To create a new scheme that is not based on an atom property, or is based on an atom property for which a scheme already exists, you can copy the scheme, by selecting it in the list and clicking Copy, and then edit it.

To edit a color scheme, select it in the list, and click Edit. The Edit Color Scheme dialog box opens, and allows you to change the scheme. If the scheme is not a standard color scheme, you can change the name in the Name text box. You can modify the description of the scheme in the Description text box.

Color schemes are defined in terms of rules, which are applied in order. The first rule has the lowest priority, and can be superseded by any of the subsequent rules. Each rule is defined by an ASL expression, and a color is assigned to that rule. The rules, their descriptions, and their colors are listed in the Rules table.

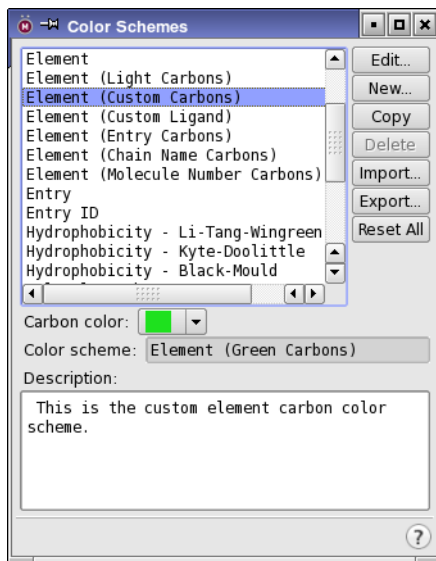


Figure 7.2. The Color Schemes panel.

- To add a new rule, click New. A new rule is added to the end of the table.
- To insert a rule after an existing rule, select the rule and click Copy. The copy is inserted after the selected rule, and the selection is moved to the copy.
- To delete rules, select the rules and click Delete.
- To revert the rules for a standard scheme to their defaults, click Reset All. This button is not available for custom color schemes.
- To change the color for a given rule, click the color cell, and choose a new color in the Choose Color dialog box.
- To set the colors for multiple rules from a color ramp, select the rules, choose the color ramp from the Color ramp option menu, and click Apply.
- To change the description for a rule, edit the table cell.
- To change the ASL expression for a rule, do one of the following:
  - Edit the ASL cell directly to change the expression
  - Right-click and choose Element, then one of the common elements.
  - Right-click and choose Residue Type, then one of the standard residues.
  - Right-click and choose Select to set up the ASL expression in the Atom Selection dialog box.

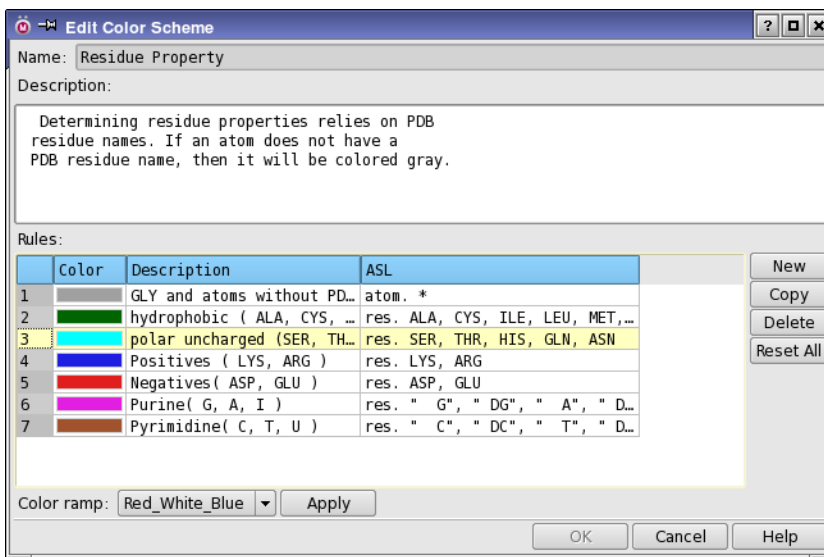


Figure 7.3. The Edit Color Scheme dialog box.

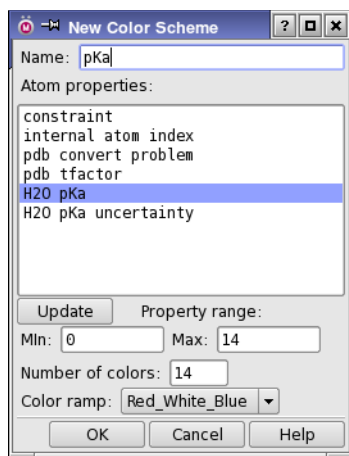


Figure 7.4. The New Color Scheme dialog box.

To preview the color scheme, you can apply it by using the tools in the Atom Color tab of the Atom and Bond Coloring panel.

To create a new color scheme from an atom property, click **New**. The New Color Scheme dialog box opens, and you can enter a name, select an atom property from the list, set the minimum and maximum values of the property for the color scheme, the number of colors to use and choose a color ramp. If you want some idea of the range of property values, include a molecule in the Workspace that has a typical range, and click **Update**. The minimum and maximum values for this molecule are entered into the **Min** and **Max** text boxes. When you have made settings, click **OK** to create the new scheme.

New or edited color schemes are stored in your [Maestro user resources directory](#). For information on color scheme and color ramp files, see [Section 13.5 on page 320](#).

You can export and import color schemes, by clicking **Export** or **Import** in the Color Schemes panel. These buttons open standard file selectors, in which you can browse to the appropriate location for the color scheme file.

To delete a color scheme, select it in the color scheme list, and click **Delete**. You cannot delete standard schemes, only custom schemes. To remove all custom schemes and revert to the standard schemes, click **Reset All**.



## 7.2.5 Setting the Background Color

The default background color of the main window is black, but the color can be changed to adjust the contrast between the background and the Workspace atoms. To change the background color, choose **Workspace** → **Appearance** in the main window and select the **Background** tab. You can set the color by clicking the color button and choosing a color in the standard color selector that opens, or you can use one of the five preset colors. The preset colors are also available from the shortcut menus in the Workspace.

## 7.3 Changing Molecular Representations

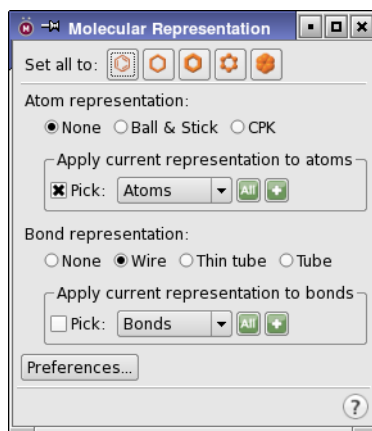
The molecular representation is the way in which atoms, bonds, and protein chains are drawn in the Workspace. Atoms can be drawn as points or as spheres, and bonds can be drawn as lines (wires) or as tubes. Protein chains can be drawn as flat “ribbons” or as tubes, representing the secondary and tertiary structure of the protein rather than the atoms.

The basic choice of the type of representation can be done in the Molecular Representation panel and the Ribbons panel, with corresponding toolbar items for the main actions. These choices are described in the sections below. The details of the rendering of these objects, as well as default choices of the type of representation and other settings, are made in the Molecular Representation settings group in the Preferences panel,—see [Section 14.13 on page 371](#).

To open the Molecular Representation panel, choose **Workspace** → **Molecular Representation**.

To open the Ribbons panel, choose **Workspace** → **Ribbons**.

These panels are dockable panels, that open by default docked in the main window. To change this behavior you can set preferences—see [Section 14.1.6 on page 335](#).



**Figure 7.5.** The Molecular Representation panel.

### 7.3.1 Changing the Representation of Atoms And Bonds

In the Molecular Representation panel, you can change the representation of atoms and bonds. These representations are not entirely independent: most of the options set both the atom representation and the bond representation.

At the top of the panel, you can set the representation for all atoms in the Workspace to one of the five main representations: wire frame (lines), thin tubes, tubes, ball and stick, or CPK (spheres). The buttons you use to set these representations are the same as on the Representation toolbar (see [Section 7.1 on page 133](#)).

Under Atom representation, you can choose between three options for the representation of atoms, with the corresponding bond representation. The options are:

- None—no representation of atoms, with bonds represented as wires.
- Ball & Stick—represent atoms as spheres, and bonds as tubes.
- CPK—represent atoms as large spheres, using the van der Waals radii of the atoms for the sphere radii. The bond representation is not changed if you set it with the Bond representation options; otherwise it reverts to wire.

To apply the atom representation, use the picking tools in the Apply current representation to atoms section to select atoms to apply the representation.

Under Bond representation, you can choose between four options for the representation of bonds, with the corresponding atom representation. The options are:

- None—no representation of bonds. This option only sets the bond representation; the current atom representation remains in effect.
- Wire—represent bonds as wires (lines), with no representation of atoms.
- Thin tube—represent bonds as thin tubes, with atoms represented by spheres the same size as the tubes (i.e. caps to the tubes).
- Tube—represent bonds as tubes, with atoms represented by spheres the same size as the tubes (i.e. caps to the tubes).

You can mix representations within a single molecule by picking. When you do so, the half of each bond that is attached to each atom that is picked is represented with the chosen bond style.

You can apply a molecular representation to atoms using the buttons on the Representation toolbar.



Click and hold any of the buttons to pick the structural unit to apply the representation to. Double-click either button to apply the representation to the selected atoms, or to all atoms if there is no selection. You can choose the structural unit to pick from the button menus.

For atoms represented in CPK, the depth view can be enhanced using an approximate calculation of ambient occlusion, which takes into account the ambient lighting that is blocked by nearby atoms. To enable the enhancement, select Enhanced depth view under Workspace – Depth view in the Preferences panel or from the Workspace menu in the main window, or press D when the pointer is in the Workspace.

### 7.3.2 Rendering Proteins, DNA, and RNA as Ribbons

In the Ribbons panel you can display protein backbones as a ribbon diagram and DNA and RNA as a ladder diagram. Displaying ribbons can simplify the analysis of secondary and tertiary structures. You can choose from seven ribbon styles and nine color schemes, and apply the ribbon style by picking or using the Atom Selection dialog box. You can mix representations within a single protein by picking.

To open the Ribbons panel, choose Workspace → Ribbons on the main menu bar.

Ribbons are defined by a style and a color scheme. The choices of style are:

- Cartoon—display loops as thin tubes, sheets as arrows and helices as ribbons.
- Ribbon—thin, curved flat surface that follows the backbone.
- Tube—curved tube that follows the backbone.
- Thin Tube—thin curved tube that follows the backbone.
- Curved Line—curved line that follows the backbone.

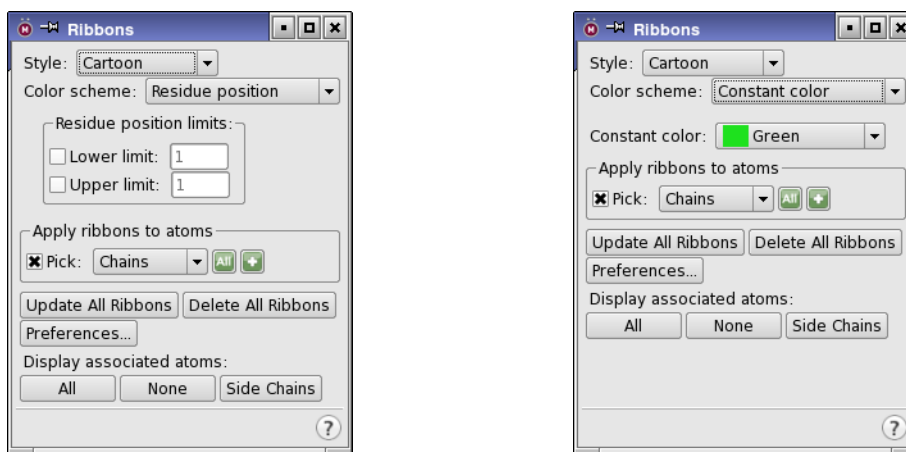


Figure 7.6. The Ribbons panel, showing tools for color schemes.

- CA Trace—straight line that connects alpha carbon atoms.
- CA Trace Tube—straight tube that connects alpha carbon atoms.

The Color scheme option menu provides a range of properties which can be used to select the color scheme, such as residue properties and secondary structure. Each of these has a predefined set of colors that is applied to the ribbon.

With the exception of the CA Atom Color scheme, the color schemes are described in the Color Scheme tab of the Atom Coloring panel (see [Section 7.2.3 on page 135](#)). In the CA Atom Color scheme, the ribbon is colored with the current color of the alpha carbon atoms. Thus, if you change the color of certain residues and reapply this color scheme, the section of the ribbon for which you changed the residue color changes color to match.

In the Ribbon or the Cartoon style, helices can be colored the same color on both sides of the ribbon, or the inside can be colored gray. The choice between these two is made by setting a preference in the Molecular Representation – Ribbons section of the Preferences panel (see [Section 14.13.2 on page 374](#)).

Two of the color schemes have other choices that you can make. The controls for these choices are displayed in the panel when you choose the color scheme—see [Figure 7.6](#)—and are described below.

- Constant color—Choose the color to use for coloring the ribbons. This option menu is only available if you choose Constant color from the Color scheme option menu.
- Residue position limits—These options allow you to set residue number limits for applying the Residue position color scheme, and are only available when that scheme is chosen from the Color scheme option menu. Residues with residue numbers outside the range are colored with the color for the end of the range. Insertion codes are ignored.
  - Lower limit—Select this option to set the lower limit for coloring, and enter the lowest residue number in the text box.
  - Upper limit—Select this option to set the upper limit for coloring, and enter the highest residue number in the text box.

To apply the chosen style and color scheme, you can use the picking tools in the Apply ribbons to atoms section. You can apply the current scheme to all existing ribbons by clicking Update All Ribbons.

You can apply the color schemes and the display options using the Ribbons toolbar button.



If you want to change the quality of the ribbons, the blending of ribbon colors, or the width or thickness of the ribbons, strands, tubes, or ladders, click Preferences. The Preferences panel opens at the Molecular Representation – Ribbons section. You can also control which of the atoms that are associated with the ribbons are displayed when ribbons are created. See [Section 14.13.2 on page 374](#) for more information.

You can change the atom visibility with the usual display tools. In addition to these, the Show, hide or color ribbons button menu offers a number of options for the display of ribbons and the associated atoms:

- Show Ribbons for All Residues
- Show Ribbons for Selected Residues
- Show Ribbons for Displayed Residues
- Select Atoms to Display Ribbons
- Display Atoms
- Undisplay Atoms
- Display Side Chains Only
- Delete Ribbons

The first three items create the ribbons for the particular choice of residues, while the fourth item opens the Atom Selection dialog box so you can choose residues for the ribbons. The next three items display or undisplay atoms associated with the ribbons.

## 7.4 Changing Lighting, Materials, and Special Effects

The lighting effects and the materials that objects in the Workspace appear to be made of can be changed in the Appearance panel, which you open by choosing Workspace → Appearance. Special effects can also be added to enhance the appearance of objects in the Workspace.

The Lighting tab of the Appearance panel contains controls for the lighting effects on objects in the Workspace. There are two available light sources, light1 and light2, which you can control independently. Maestro normally only uses one light source. To edit the parameters for one of the light sources, select it in the list, and then select Use light if it is not selected. The controls then become available.

The Light direction control allows you to pick the direction of the selected light, and also displays the parameters that you set. To change the direction, click the desired location on the red ball, or drag the yellow spot to the desired location.

You can change three parameters of the lighting of objects in the Workspace. Each parameter has a slider and a text box.

- Ambient—Set the intensity of the ambient (nondirectional) light. This value affects the shade of the object on the side away from the light source. A value of 100 means that there are no shadows.
- Diffuse—Set the intensity of diffuse (nondirectional) reflection from the object. and text box. A value of zero means that there is no (or minimal) reflection from the object, and so it appears to be dark.
- Specular—Set the intensity of the specular reflection (“highlight”) of the object. The highlight is essentially the image of the light source, diffused somewhat by the material of the object. To change the character of the specular reflection, use the controls in the Materials tab.

You can restore the default values for a light source by clicking Restore Defaults.

The Materials tab contains controls for the definition of the appearance of the objects in the Workspace. You can set the appearance characteristics of different object types: atoms and bonds, ribbons, surfaces, hypotheses, Phase QSAR objects. To make settings for one of these object types, first choose the type from the Object type option menu, then make the settings.

There are four preset material types, given in the Preset section: Metallic, Plastic, Rubber, Wood. These material types correspond to particular settings of the five parameters in the Custom section.

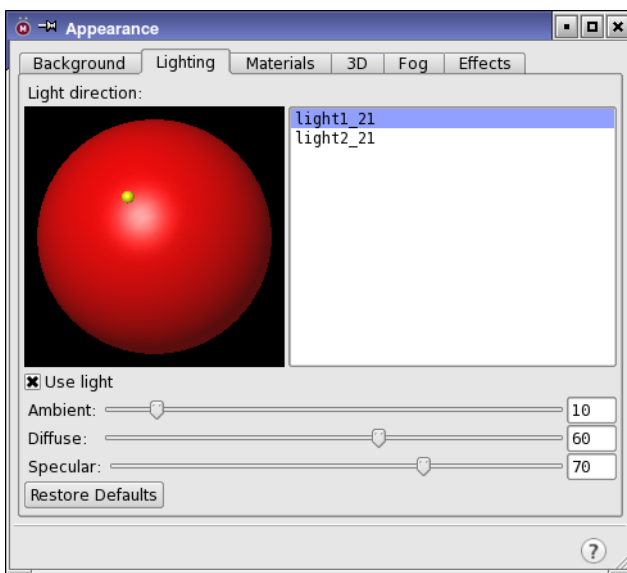
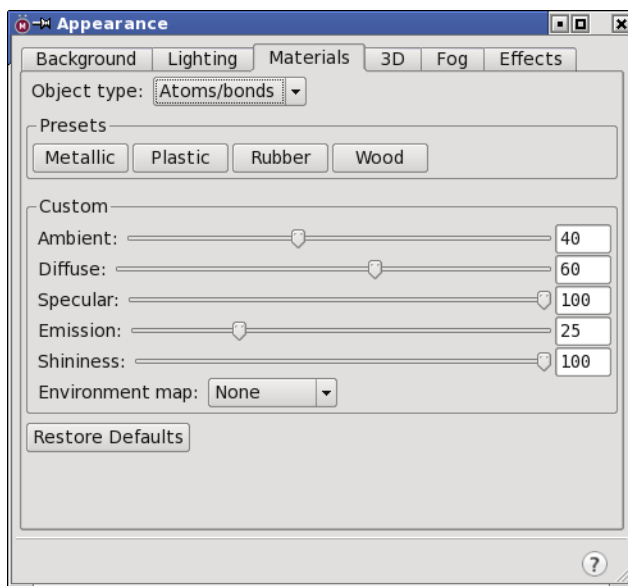


Figure 7.7. The Lighting tab in the Appearance panel.



**Figure 7.8.** The Materials tab in the Appearance panel.

The Custom section allows you to set the five properties of the material:

- Ambient—Intensity of the ambient (nondirectional) lighting
- Diffuse—Intensity of diffuse (nondirectional) reflection
- Specular—Intensity of specular reflection (the “highlight”)
- Emission—Intensity of nondirectional light emission from the object
- Shininess—Size and brightness of the highlight (specular reflection). Larger values produce a smaller and brighter highlight.

Each property has a slider and a text box. You can use either of these controls to set the property value. Setting of all five parameters has a performance cost, because there is a balance between them. The Minimize performance cost option disables the Ambient and Diffuse controls, and uses these properties to track color. This option is only present for OpenGL level 1.2, as the performance cost for 2.1 is negligible.

The Environment map option menu provides a selection of environments (“pictures”) that are shown as reflections on the surfaces of the objects in the Workspace. This menu is only present when the OpenGL level is 2.1.

You can restore the default material values for an object by clicking Restore Defaults.

Some combinations of lighting and material are available from the Style toolbar—see [Section 7.6 on page 153](#).

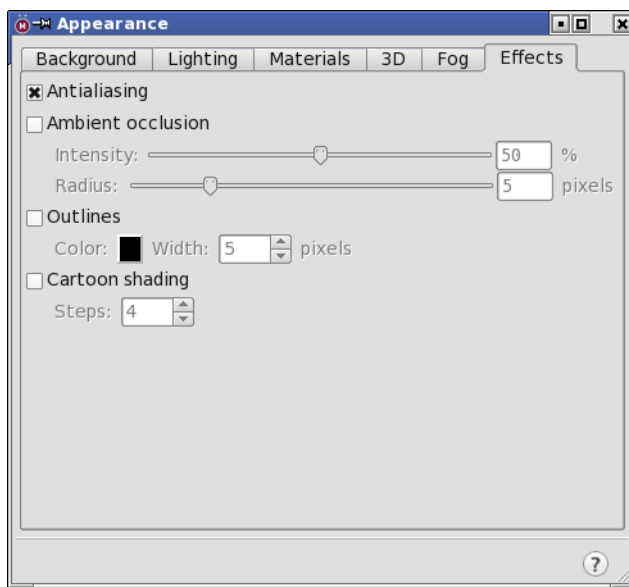


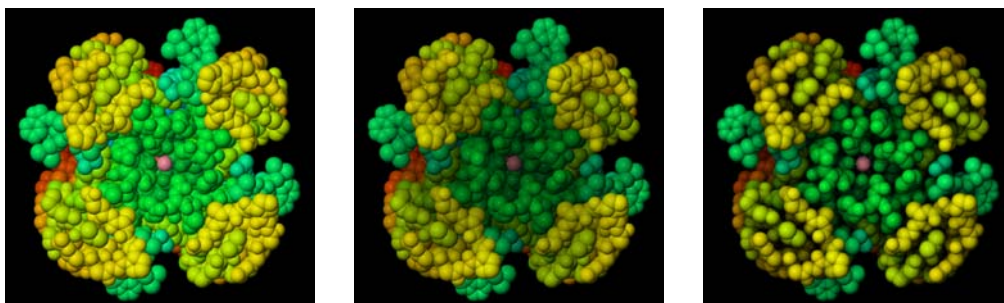
Figure 7.9. The Effects tab in the Appearance panel.

Special effects can be added to structures in the Effects tab. There are four effects available, which can be combined. These effects apply to the entire screen (Workspace). Other effects can be added to specific objects, as highlights—see [Section 8.5 on page 168](#). Some of the screen effects are also available as preferences, though with limitations. The effects are:

- Antialiasing—smooth the edges of objects so they don't appear jagged. This effect does not antialias semi-transparent objects. The Full-scene antialiasing preference ([Section 14.4.16 on page 351](#)) does, but it does not antialias spheres and cylinders (balls and sticks). For the smoothest edges, use both the preference and the screen effect.
- Ambient occlusion—enhance the perception of depth by taking into account the ambient lighting blocked by nearby objects, pixel by pixel. The Enhanced depth view preference ([Section 14.4.12 on page 350](#)) uses ambient occlusion based on atoms, and is only available for structures in CPK representation. This option is most useful for large structures in CPK representation and with molecular surfaces.

You can set the intensity of the darkening effect with the Intensity slider and box. The intensity is represented as a percentage, with 0 corresponding to no effect. You can also change the range of the effect, with the Radius slider and box. Any screen object within the specified radius of a pixel is considered to occlude the pixel. Thus, the smaller the radius, the more local and “sharp” the effect. At a very small radius, the effect is like outlines.





**Figure 7.10.** Use of ambient occlusion. From left to right: no effect, Enhanced depth view preference (atom based), Ambient occlusion screen effect (pixel-based).

- Outlines—Add a thin outline to objects in the Workspace. You can set the width of the outline (in pixels) in the Width text box, and you can set the color with the color button.
- Cartoon shading—Use cartoon shading, in which the color or shading is done in steps rather than continuously. You can set the number of steps in the Steps text box.

This tab is not present if the OpenGL level is 1.2, as it requires features that are not present at this OpenGL level.

## 7.5 Displaying and Undisplaying Atoms

Maestro provides a range of tools for selectively displaying or undisplaying atoms. These tools are available in the Display/Undisplay Atoms panel, on the Display toolbar, and on the Selection shortcut menu. Maestro also provides tools for displaying atoms that are related by crystallographic symmetry and alternate positions for atoms.

### 7.5.1 The Display Atoms Toolbar

Many of the operations for displaying or undisplaying atoms are available from the Display Atoms toolbar, and some of them are only available from the toolbar. The toolbar buttons are described in brief below, and their use is described in the following sections.



#### Display Sel

Display only the selected atoms. This button has a menu from which you can choose a structural unit to use when picking atoms for display. Choose a structural unit, then click on an atom to display the atoms in that unit only. Double-click to display only the selected atoms, or all atoms if there is no selection.



#### Display Only

Display only the atoms in a particular category. From the button menu, you can select a category of atoms to display, or open the Atom Selection dialog box to select atoms to display.



#### Also Display

Add the atoms in a particular category to the display. From the button menu you can select a category of atoms to add to the display, or open the Atom Selection dialog box to select atoms to add to the display.



#### Undisplay

Undisplay (hide) atoms in a particular category. From the button menu you can select a category of atoms to undisplay, or open the Atom Selection dialog box to select atoms to undisplay.



#### Within

Display residues within a specified distance of the currently displayed atoms. Entire residues that have any atoms within this distance of the displayed atoms are added to the display. From the button menu you can select a specific distance, or open a dialog box to enter a distance. Clicking the button performs the action.

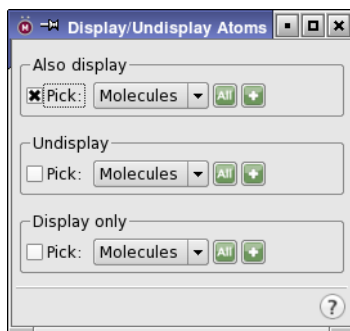
## 7.5.2 Selectively Displaying Atoms

You can display or undisplay (hide) atoms using the toolbar buttons or the Display/Undisplay Atoms panel. These tools allow you to select the atoms that are displayed or are not displayed in the Workspace. For example, you can hide from view all atoms, user-defined atom subsets, or predefined subsets such as protein backbones, side chains, water molecules, or hydrogen atoms.

Displaying and undisplaying atoms is not the same as including or excluding entries from the Workspace: it is merely changing the visibility of the atoms that are part of entries included in the Workspace. The display state is stored with the project entry, so when you include it in the Workspace later on, the same atoms are displayed or hidden. Undisplaying atoms is not the same as deleting atoms, which removes them from the project entry.

To open the Display/Undisplay Atoms panel, choose Display/Undisplay Atoms from the Workspace menu (see [Figure 7.11](#)).

The Display/Undisplay Atoms panel is divided into sections for the following three operations.



**Figure 7.11.** The Display/Undisplay Atoms panel.

- Also Display—add the selected atoms to the atoms that are already displayed.
- Undisplay—do not display the selected atoms.
- Display Only—display only the selected atoms.

You can choose the atoms for the operation using the picking tools. You can also pick atoms to display using the Display Sel button on the toolbar:

You can apply the display operation to a range of common atom groups using the Atom Selection button.



The common atom groups are also available from the toolbar on the Display Only, Also Display, and Undisplay button menus:



You can also choose Select from these button menus to open the Atom Selection dialog box and select the atoms to display or undisplay. If you already have a selection that includes atoms that are not displayed, you can add the molecules or residues that are included in this selection by choosing Display → Molecules or Display → Residues from the selection shortcut menu.

As a special case of adding to the display, you can add atoms to the display that are within a given distance of the displayed atoms, by using the Display residues within N Å of currently displayed atoms toolbar button menu:



This button menu offers a selection of distances, and a Custom item that allows you to set the distance in a dialog box. All atoms in residues that have any atom within the specified distance are added to the display, except for nonpolar hydrogens. If you want nonpolar hydrogens to be displayed as well, you can set a preference under Workspace – Display/undisplay atoms in the Preferences panel.

If you want to display atoms within a given distance of a selected set of atoms, rather than the entire displayed set, you can choose the distance from the Display submenu of the Selection shortcut menu. To display only the selected atoms and those within a given distance, choose the distance from the Display Only submenu of the Selection shortcut menu.

### 7.5.3 Displaying Periodic Structures

Structures that have periodic boundary conditions and crystal symmetry are usually only stored as the asymmetric unit—the smallest structure that can be replicated with the space-group symmetry operators to generate the entire crystal. By default, only the asymmetric unit is displayed in Maestro, but you can display replicas and other information about the periodic structures. The structures must have the unit cell parameters as entry properties. These properties are automatically added when you import a PDB structure.

Maestro can display atoms that are related by crystal symmetry—“crystal mates”—for structures whose unit cell parameters are available as entry properties. The crystal mates are the nearest-neighbor replicas of the structure in the displayed entry. Display of crystal mates can be limited to a certain radius of the displayed entry. All residues in the crystal mates that have atoms within this radius of the displayed entry are displayed.

- To display all crystal mates, choose All from the Crystal Mates submenu of the Workspace menu.
- To display crystal mates within one of four predetermined radii, choose Within *radius* from the Crystal Mates submenu of the Workspace menu.
- To turn off the display of crystal mates, choose None from the Crystal Mates submenu of the Workspace menu.

Some protein structures have alternate positions for atoms—for example, when the structure contained ligands bound at two different sites, or bound in different conformations. These are represented as partial occupancies. Maestro reads the alternate positions and stores them as entry properties. You can display the alternate positions of the atoms by choosing Workspace → Alternate Positions, or choosing Display Alternate Positions from the Selection shortcut menu. The alternate positions are displayed as “ghost” atoms. If you want to make the alternate positions the main positions, select the atoms, then choose Switch Alternate Positions from the Selection shortcut menu.

If you are editing a structure with alternate positions, you can set a preference for whether the alternate positions are transformed along with the main positions—see [Section 14.4.6 on page 346](#) for more information.

If you have a crystal structure whose asymmetric unit consists of a small number of atoms (50 to 100), you can use the Periodicity toolbar to display the entire unit cell and multiple surrounding unit cells, display cations surrounded by anions as polyhedrons, show bonding information, and calculate properties of the unit cell. The toolbar is described below.



#### Unit cell

Draw the unit cell boundaries or the lattice vectors, or both, in the Workspace. The choice of what to draw and the appearance can be set in the Preferences panel, under Workspace – Periodicity.



#### Show Atoms

Choose options for which atoms are shown in the Workspace and how they are shown, from the button menu. You can show the symmetry-unique atoms of the unit cell (Symmetry Unique Atoms) or all atoms in the unit cell (All Atoms). When displaying all atoms, select Intact Molecules to extend connected fragments beyond the unit cell boundaries. If you only want to see atoms that are inside a single unit cell, you can select Keep Edge Atoms to display the same atom on both sides of the unit cell, if the atom is on a unit cell boundary.



#### Calculate Bonds

Show the connectivity of the structure, displayed as single bonds. Two atoms are considered connected if the distance between them is smaller than the sum of their covalent radii plus an offset. No account is taken of bond order in the display. Clicking the button or choosing Display Bonds from the button menu displays the connectivity. Choosing Update Bonds updates the connectivity by reapplying the distance criterion. Dynamic Bonds updates the connectivity after each change in the Workspace. To adjust the distance offset, choose Options.



#### Extents

Display replicas of the unit cell along the lattice vectors. Choose Edit from the button menu to set the number of replicas in the positive and negative directions for each lattice vector, in the Edit Extents dialog box. The default is zero replicas. Choose Display Extents from the button menu to display the replicas. You must also choose All Atoms from the Show Atoms button menu to display the replicas.



#### Polyhedrons

Display polyhedrons for cations that are surrounded by 4 to 8 anions. An atom is considered as an anion if it is from Group 16 or Group 17 and has a zero or negative formal charge, or if it is N with a negative formal charge. An atom is considered a cation if it is not an anion and has a zero or positive formal charge, and has 4 – 8 bonded neighbors, all of which are anions. The color and opacity can be set in the Preferences panel, under Workspace – Periodicity.



#### Properties

Calculate unit cell properties (density, volume, and molecular formula) and add these properties to the Project Table. Opens the Project Table panel, and scrolls to these properties.

## 7.6 Display Styles

The previous sections in this chapter describe the tools that are available for changing the appearance of the structures in the Workspace. It is often the case that you want to apply more than one of these tools to your structure, and you prefer certain display attributes for all structures. You might also want to apply different display attributes to ligands and proteins. Maestro provides tools for creating a display “style”, on the Style toolbar.

The Style toolbar allows you to create and apply visual styles for the Workspace contents. The toolbar also provides easy access to the display of H-bonds and contacts, and generation and display of molecular surfaces. The style settings made with this toolbar are designed to add only those components specified, and leave any other style choices as they are. All style settings are stored as preferences, so that they persist across Maestro sessions.

The Workspace style is a set of choices for the molecular representation and color scheme of a number of entities: the ligand, waters, ions, and default settings for all other atoms. It also includes settings for the display of waters and hydrogens, and for creating receptor and ligand surfaces. The ligand is detected automatically with settings made in the Ligand Detection Settings dialog box—see [Section 7.6.3 on page 159](#).

A brief description of the Style toolbar buttons is given below, and the use of the styles is elaborated in the following subsections.



### Apply

Set and apply a defined style to the Workspace atoms. Click to apply the style, click and hold to display a menu for making style settings and ligand detection settings.

Menu equivalent: Workspace → Style → Apply Style.



### Reapply

When the Workspace content changes, reapply the Workspace style, according to the options set in the Workspace Style Settings dialog box.

Menu equivalent: Workspace → Style → Reapply Style.



### Surfaces

Create molecular surfaces for the binding site (receptor, ligand, or both) by clicking this button; show or hide surfaces or open the Surface Table panel from the button menu.

Menu equivalent: Workspace → Style → Create Binding Site Surfaces.



### Fix

Fix the receptor entry in the Workspace.

Menu equivalent: Workspace → Style → Fix Receptor.



### Rendering

Set the priority for Workspace rendering, between best quality and best performance.

Menu equivalent: Workspace → Style → Rendering.



### Material

Select combinations of material and lighting to produce a particular appearance of molecular representations and surfaces.

Menu equivalent: Workspace → Style → Material.

## 7.6.1 Applying the Workspace Style

The Workspace style is applied by clicking the Apply button:



or by choosing Workspace → Style → Apply Style. If you change the contents of the Workspace (add or remove atoms by any means: inclusion, building, deleting), the style is not automatically applied to any new atoms. If you want to apply the style whenever new atoms are added, click the Reapply button.



When this button is selected, the current style settings are applied to atoms that are added to the Workspace, subject to the settings for applying the style. Selecting this button allows you to keep the same style in effect as you change what is displayed in the Workspace. This button is deselected when you close a project, subject to a preference (see [Section 14.2.1 on page 336](#)).

There is no “undo” operation for the application of the Workspace style.

Settings for color and representation are stored with entries, so the style for any entry you include in the Workspace is changed when you apply the style. If you don’t want to change these settings, ensure that Reapply When Workspace Changes is not selected.

The style settings do not include material and lighting effects, but you can choose from a few preset styles from the Material button menu.



As well as applying a defined style, you can change the rendering, to optimize it for speed when you change the structure or the view, or for quality, which can be a little slower, or a balance between the two. You can make these choices from the Rendering button menu.



## 7.6.2 Defining the Workspace Style

The Workspace style consists of settings in three categories: molecular representation, color scheme, display of hydrogens, and a collection of “general” settings, for hiding waters, fitting to the ligand, and setting the scope of the style when the Workspace changes. The style is set up in the Workspace Style Settings dialog box, which you open by choosing Workspace → Style → Style Settings or choosing Settings from the Apply button menu.



The General tab provides overall control of what changes when the style is applied or the Workspace changes.

To adjust the zoom to fit the ligand to the Workspace when the style is applied, select Fit to ligand. The clipping settings are applied when zooming in on the ligand.

If you want to hide waters that are far from the ligand, choose the condition for undisplaying waters from the Undisplay waters option menu. The three distance options are distances from the ligand. The default is to undisplay all waters.

You can also choose how the style is applied when the content of the Workspace changes., under When Workspace changes. If you do not want the style to be reapplied, ensure that Apply settings to is not selected. If you want to reapply the style, select this option, and choose one of the two options that determine the scope of the changes:

- Entire Workspace—Apply the style settings to all atoms in the Workspace.
- Ligand only—apply the style settings only to the ligand, and not to the rest of the Workspace. This option is useful if you are stepping through ligands with a fixed receptor (such as when viewing docked poses), and it makes the updating of the Workspace faster.

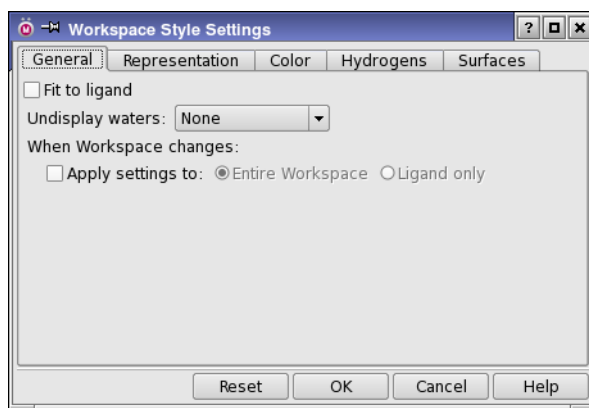


Figure 7.12. The General tab of the Workspace Style Settings dialog box.



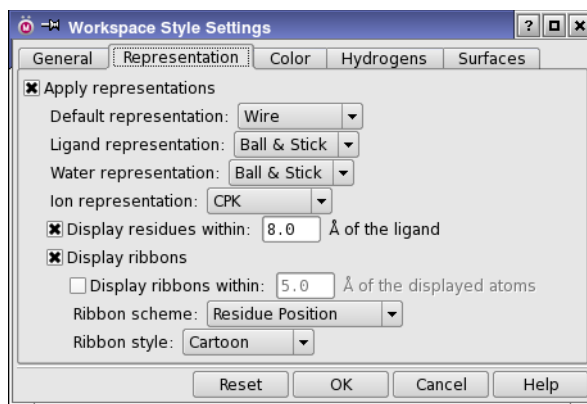


Figure 7.13. The Representation tab of the Workspace Style Settings dialog box.

In the Representation tab, you can choose the representation for the default atoms, the ligand, waters, and ions, from Wire, Tube, Thin Tube, Ball & Stick, and CPK. You can also make settings for the ribbon visibility, scheme, and style for the receptor. Other attributes are inherited from the settings in the Molecular Representation panel (see Section 7.3 on page 141). The default values are listed in Table 7.2.

If you want to see only those residues within a given distance of the ligand, select Display residues within  $N$  Å of the ligand and enter the distance in the text box.

You can choose whether or not the representation is changed when the Workspace style is applied by selecting or deselecting Apply representations. Likewise, you can choose whether to display ribbons by selecting or deselecting Display ribbons. The Apply representations option applies to ribbons as well, so the Display ribbons option only determines whether ribbons are included in the representation.

Table 7.2. Default Workspace Style settings.

Atom type	Representation	Color Scheme
Default	Wire	Element
Ligand	Ball & Stick	Element (Entry Carbons)
Water	Ball & Stick	Element
Ion	CPK	Element

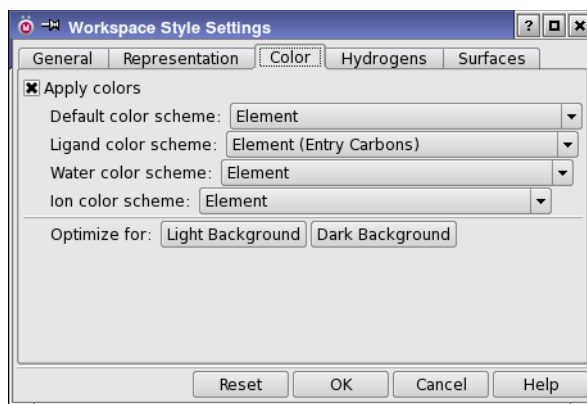


Figure 7.14. The Color tab of the Workspace Style Settings dialog box.

In the Color tab, you can choose the color scheme to use for each of the four entities. The color schemes are described in Table 7.1, and the defaults are listed in Table 7.2. The Optimize for buttons make a particular selection of color schemes, optimized for a light background or a dark background. You can choose whether or not the color schemes are changed when the Workspace style is applied by selecting or deselecting Apply colors.

In the Hydrogens tab, you can choose which hydrogens to display for the receptor and for the ligand. The choices are None, Polar only, and All. The default for the receptor is Polar only, and for the ligand is All.

In the Surfaces tab, you can choose whether to generate surfaces for the receptor (Create receptor surface) or the ligand (Create ligand surface) or both when the Workspace style is applied. This includes application when the Workspace changes, if you have the option set in

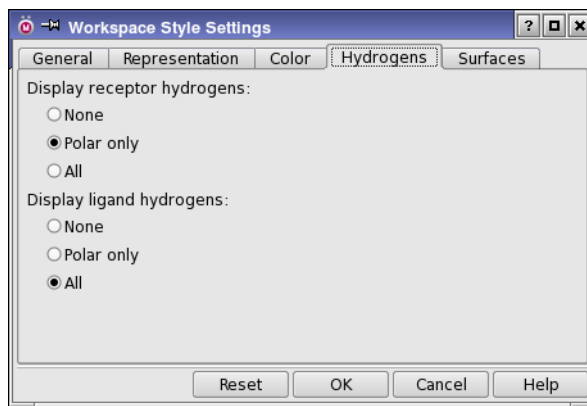


Figure 7.15. The Hydrogens tab of the Workspace Style Settings dialog box.

the General tab. The surfaces are generated according to the settings in the Create Binding Site Surfaces dialog box. These two options create surfaces every time the style is applied, and delete the previous surfaces and any related volumes. This might take some time.

You can manually create surfaces as well—see [Section 7.6.4 on page 160](#)). The manually created surfaces are stored independently.

### 7.6.3 Ligand Detection

An important feature of the style settings is automatic detection of the ligand. The criteria by which the ligand is detected can be set in the Ligand Detection Settings dialog box, which you open by choosing Ligand Detection Settings from the Apply toolbar button menu.



In the Ligand molecules section, you can set size limits on the ligand molecule, by specifying the minimum and maximum number of atoms that a ligand molecule can have. There are two options to cover special cases: Allow molecules that are small ions, and Allow molecules containing only amino acids. By default, small ions and small peptides are excluded from consideration as ligand molecules.

In the Excluded residues section, you can select from a list of molecules that commonly appear in biological systems, to exclude them from consideration as ligands. By default, all these residues are excluded. To allow a residue to be considered as a ligand, deselect the check box in the Exclude column for that residue. You can also add your own molecules, by specifying the

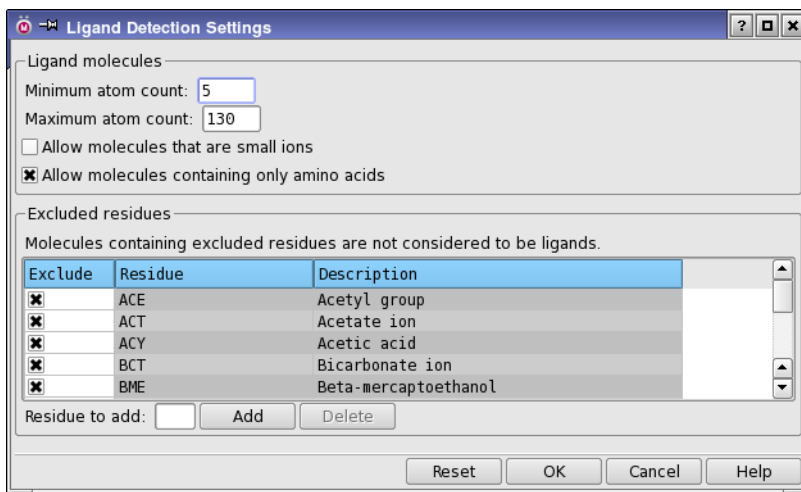


Figure 7.16. The Ligand Detection Settings dialog box.

residue code in the Residue to add text box and clicking Add. The code can be up to 4 letters long. You can delete residues by selecting them in the table and clicking Delete. The exclusion is done by checking for the residue code, not by any structural matching.

To restore the default ligand detection settings, including the standard list of excluded residues, click Reset.

## 7.6.4 Surfaces

Another feature of the Workspace style toolbar is the ability to create and display molecular surfaces for the binding site. The surfaces can be set up manually by clicking the Create Binding Site Surfaces button



or by choosing Workspace → Style → Create Binding Site Surfaces or Workspace → Surface → Create Binding Site Surfaces. In the Create Binding Site Surfaces dialog box, you can choose whether to create surfaces for the ligand, the receptor, or both, by choosing the appropriate options. You can control the extent of the receptor surface from the ligand, the transparency and the grid spacing (surface quality), the surface style, and the color scheme. To restore the default values, click Reset.

When you have created the surfaces, you can display or hide all of them from the Create Binding Site Surfaces button menu:



If you want greater control over which surfaces are displayed and how they are displayed, choose Manage from this button menu, or choose Workspace → Surface → Manage Surfaces, to open the Manage Surfaces panel. This panel is described in detail in [Section 12.4 on page 305](#). See [page 158](#) for information on automatic creation of surfaces.

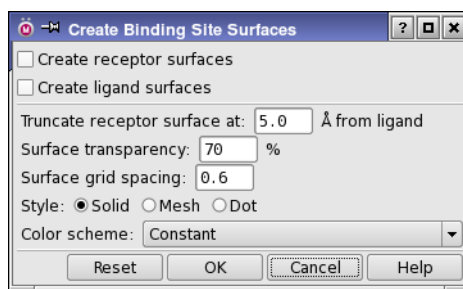


Figure 7.17. The Create Binding Site Surfaces dialog box.

# Labeling and Annotating the Workspace

Maestro has several ways that you can annotate the Workspace and its contents, by adding text or highlights. Text can be added as atom labels, as captions, or as project entry information (“feedback”). Highlighting of atoms can be done with changes in color intensity or contrast, or by adding a silhouette, and can include text with an arrow pointing to the highlight.

## 8.1 The Labels Toolbar

All of the annotation methods can be applied by using the Labels toolbar, which you can display from the Manager toolbar, or by choosing Window → Toolbars → Labels. The toolbar buttons are described in brief below, and their use is described in the following sections.



### Label All

Label all atoms (or target atoms) with the selected label. This button has a menu from which you can select and apply the label, set the current label composition, delete labels, and select an option to reapply the labels when the Workspace changes. The target atom is the first atom in an entry or the C $\alpha$  atom of a residue if entry or residue properties are used in the label. All atoms are labeled if an atom property is used in the label.



### Pick to Label

Pick atoms in the Workspace to apply a label. From the button menu you can:

- choose a structural unit to use when picking atoms for labeling
- open the Atom Selection dialog box to select atoms to label
- compose labels in the Atom Labels panel
- reset label positions
- set label preferences
- delete labels

Double-click to apply the label to the selected atoms, or to all atoms if there is no selection.



### HBonds

Display hydrogen bonds as yellow dotted lines. This button has a menu from which you can choose to display H-bonds between entries (*Inter*) or within entries (*Intra*), or both (*All*); open the Preferences panel to make settings for H-bonds; and delete H-bond markers.



### Measure

Measure distances, angles, dihedrals or NMR coupling constants. From the button menu you can choose between distance, angle, dihedral, or <sup>1</sup>H NMR coupling for measurement, open the Preferences panel to make settings for measurements, or delete measurements.

Menu equivalent: Tools → Measurements → Pick to Measure.



#### User Text

Change the user-defined text in the atom label on the picked atom. If the atom does not have a label, a label is added. A dialog box opens, to enter the text and choose whether to replace the entire label or replace the text in the label.



#### Feedback

Display information about a single entry, termed the “target” entry, in the top left corner of the Workspace.

Menu equivalent: Workspace → Single-Entry Feedback.



#### Highlights

Create, modify, delete, or apply highlights to atoms in the Workspace. Opens the Manage Highlights panel.

Menu equivalent: Workspace → Highlights.



#### Quick Highlight

Add a highlight to picked atoms with the current highlight settings. From the button menu you can choose a structural unit for picking to highlight; open the Atom Selection dialog box to select atoms to highlight; or open the Manage Highlights panel to make highlight settings.



#### Add Caption

Add a caption to the Workspace. Opens the New Caption dialog box, in which you can type in the text, and set the caption background, font, and text color.

Menu equivalent: Workspace → Add Caption.



#### Show Cap

Show or hide the Workspace captions.



#### Increase Fonts

Increase the size of all the Workspace fonts (atom labels, measurements, adjustments, captions, highlights, feedback).



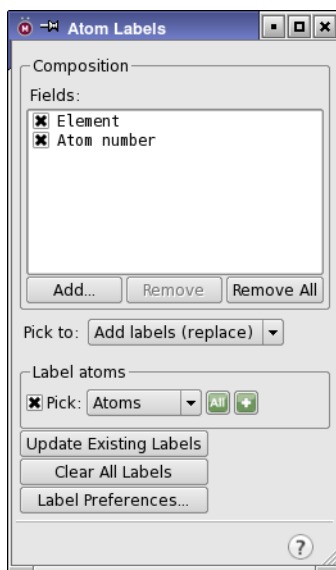
#### Decrease Fonts

Decrease the size of all the Workspace fonts (atom labels, measurements, adjustments, captions, highlights, feedback).

## 8.2 Labeling Atoms

Labels are useful tools for building, identifying, and analyzing molecular structures since they can be used to display any combination of predefined information or user-specified text. For instance, you might want to display atom numbers so that you can retype a specific atom, or to pick atom pairs for superposition, inclusion in a set, or measurement.

Atom labels are persistent. The labels are stored as part of the entry, and are restored when an entry is excluded from then included in the Workspace. However, labels that are dependent on the numbering in the Workspace, such as Molecule Number, may change because they are relative to the Workspace, not the entry.



**Figure 8.1. The Atom Labels panel.**

Labels can be set up and applied in the Atom Labels panel. To open the Atom Labels panel, choose *Workspace* → *Atom Labels* or choose *Composition* from the *Label All* or the *Pick to Label* button menu.

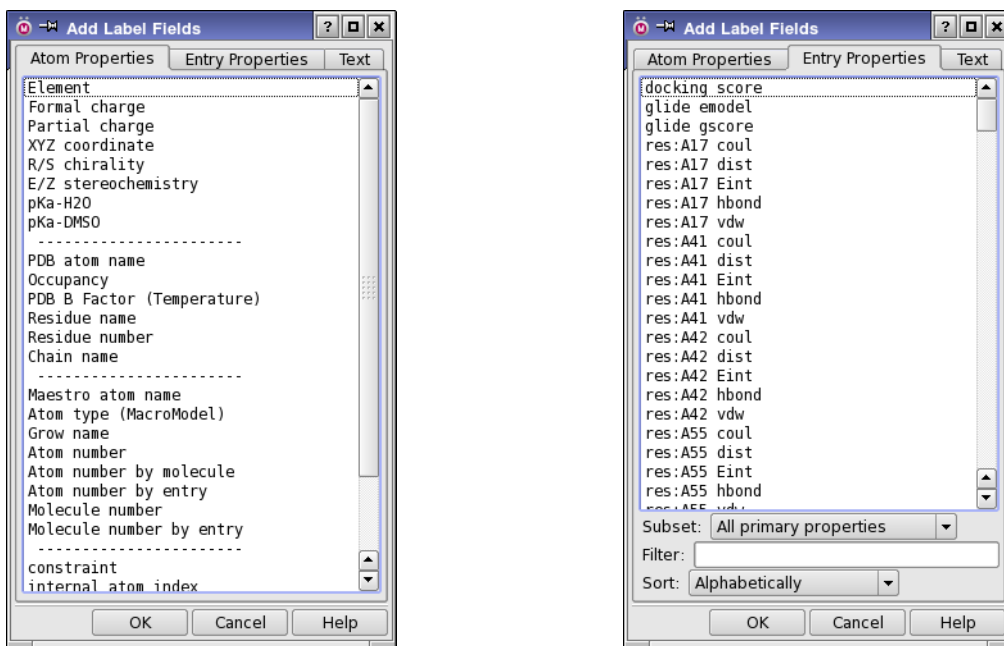


Labels can be constructed from a variety of atom, molecule, residue, chain, and entry properties, including element, charge, stereochemistry, atom and residue names and numbers, and also user-defined atom and entry properties. By default, the *Element* and *Atom number* atom properties are in the label.

To add properties to the label composition, click *Add*, and select the properties in the *Add Label Fields* dialog box. The *Atom Properties* and *Entry Properties* tabs have lists of properties that you can select. You can filter and sort the entry properties. Click *OK* to add the selected properties to the label composition.

To remove properties from the label composition, select them in the *Fields* list, and click *Remove*. To remove all properties, click *Remove All*.

To show or hide properties in the label, but keep them in the list for easy access, check or clear the check box for the properties. This allows you to keep the properties that you want to use most often for labels available, but quickly change the displayed label.



**Figure 8.2. The Add Label Fields dialog box, Atom Properties tab (left) and Entry Properties tab (right).**

The properties are added to the label in the order they appear in the Fields list. You can change this order by selecting properties in the list and dragging them to the desired position in the list. The property values are separated by spaces in the label.

When you have finished composing the label, choose Add labels (replace) from the Pick to option menu to begin adding labels.

To select the atoms for the chosen labeling action, use the standard picking tools in the Label atoms section. Labels are added to atoms that do not have labels, and existing labels are replaced on atoms that already have labels. The labels are applied only at the time you perform the labeling action, and do not change if you change the composition. If you want to update all labels with the new composition, click Update Existing Labels.

If you want to remove labels, you can do so by selecting atoms or you can remove all labels. To select atoms to remove labels, choose Clear labels from the Pick to option menu, then use the standard picking tools in the Label atoms section. To remove all labels, click Clear All Labels.



To label atoms with your own text, click the User Text button on the Labels toolbar:



then pick the atom in the Workspace. The User Text dialog box opens, in which you can enter the text, and choose whether to show only the text you entered (Only this text), or add the user text to the label, replacing any existing user text (This text in label). You can also pick the atom first, then click the button. User text is added to the Composition list, and can be turned on and off like any other property in the label.

You can label atoms from the Labels toolbar. To apply labels for a single property from a subset of the full range of properties (or the current label composition), choose the property (or Current Composition) from the Label All button menu on the Labels toolbar:



The labels are applied to all atoms, if the property is an atom-level property. If it is a residue property, the label is applied to the alpha carbon. If it is an entry property, it is applied to the first atom in the entry.

This button menu also has a Reapply atom labels when Workspace changes option, which reapplies the label that was selected from the button menu whenever the Workspace content changes. You can also reapply the label manually by clicking the button.

To apply the current labeling scheme by picking, use the Pick to Label button menu:



Double-click this button to apply the current labeling scheme to all atoms. From the button menu you can choose Composition to open the Atom Labels panel with the Composition tab displayed, you can choose Select to open the Atom Selection dialog box to select the atoms to label, and you can choose Delete Labels to delete all labels.

You can customize the appearance, formatting, position, and behavior of all labels in the Atom/Bond label group in the Preferences panel. To open the Preferences panel at the Atom/Bond label group, click Label Preferences in the Atom Labels panel or choose Label Preferences from the Pick to Label button menu. See [Section 14.6 on page 355](#) for more information.

To reposition an individual label, drag the label to the desired location. To restore an individual label to its default location, right-click on it and choose Reset Position. If you want to reset all labels to their default positions, choose Reset Positions from the Pick to Label button menu.

## 8.3 Labeling Bonds

Like atoms, bonds can be labeled with bond properties. The bond property must be a property of the entry, not something like a distance measurement. Bond properties are added to structures by some applications, and you can use these to label bonds.

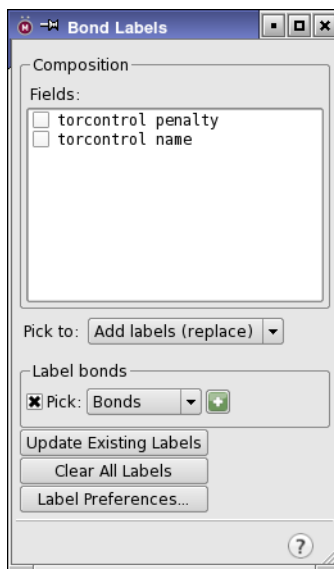
Bond labels can be set up and applied in the Bond Labels panel. To open the Bond Labels panel, choose *Workspace* → *Bond Labels*. The properties to include in the label can be selected in the *Fields* list, which shows all bond properties in the project.

When you have finished composing the label, you can apply the labels. There are two labeling actions that are applied by selecting bonds, which you choose from the *Pick to* option menu:

- **Add labels (replace)**—Add labels to the selected bonds, replacing any existing labels.
- **Add labels (append)**—Add labels to the selected bonds, appending to any existing labels.

To select the bonds for the chosen labeling action, use the standard picking tools in the *Label bonds* section. The labels are applied immediately. If you want to update all bond labels with the new composition, click *Update Existing Labels*.

If you want to remove the labels, you can do so by selecting bonds, or you can remove all labels. To select bonds to remove labels, choose *Clear labels* from the *Pick to* option menu, then use the standard picking tools in the *Label bonds* section. To remove all labels, click *Clear All Labels*.



**Figure 8.3.** *The Bond Labels panel.*

Bond labels can be repositioned by dragging. To revert to the default position, right-click on the label and choose Reset Position.

The formatting of the label (font, color, position) can be set as preferences—see [Section 14.6 on page 355](#). Atom labels and bond labels share most of the preferences, but the bond label color can be set independently.

## 8.4 Captions

Captions can be used to display any kind of text in the Workspace, in a text box. They are stored as part of the project.

To create a caption, either choose Workspace → Add Caption, or click the Add Caption button on the Labels toolbar.



The New Caption dialog box opens. Enter the caption text in the Workspace caption text area (including any line breaks), choose the background style (transparent or automatic contrast to the text), font attributes, and color, and click OK. The caption is displayed in the Workspace. The gray border indicates that it is selected: it is not part of the caption. You can drag the caption to the desired location.

The caption size is determined by the size of the text and the font. It does not change when you zoom in and out. The shape of the caption is determined by where you place line breaks in the text that you enter.

If you want to change the text of a caption, double-click on the caption, or right-click on the caption and choose Edit Caption. You can then make changes in the Edit Caption dialog box, which has the same controls as the New Caption dialog box.

You can select one or more captions in the Workspace with shift-click and control-click. Selected captions are displayed with a gray border. You can reposition the selected captions as a group by dragging them. To delete them, you can press Delete, right-click and choose Delete Selected Captions from the shortcut menu, or choose Captions from the Delete button menu on the Edit toolbar.



To show or hide the captions, you can use the Show Cap button on the Label toolbar.



## 8.5 Highlights

Highlights are graphical annotations of a set of atoms in the Workspace, with optional text annotation. The sets of atoms are defined by ASL expressions, so the highlight can be applied to different entries that have a match to the ASL expression.

There are three types of highlight:

- **Silhouette**—A colored border of a specified thickness is drawn around the atoms and bonds.
- **Contrast**—The brightness of the non-highlighted atoms is reduced. At 100% contrast, these atoms are no longer visible.
- **Saturation**—The color saturation of the non-highlighted atoms is reduced.

Each of these three types of highlight can have associated text and an arrow pointing to the highlight.

Highlights can be created, edited, and deleted in the Manage Highlights panel, and are stored with the project. To open the Manage Highlights panel, choose *Workspace* → *Manage Highlights*, or click the Highlights button on the Labels toolbar.



You can also choose *Settings* from the Quick Highlight button menu on the Labels toolbar to open the panel.

### 8.5.1 Creating and Editing Highlights

To create a highlight, click *New*. A dialog box opens, in which you can name the highlight. The highlight is listed in the table at the top of the Highlights tab, and the highlight is selected in the table.

After you have created a highlight, you can choose a highlighting method from the *Method* option menu in the *Atoms* tab, then use the Highlight atoms picking tools to pick the atoms to highlight.

Picking atoms in the Workspace creates a highlight that is specific to the entry whose atoms you picked. If you want a highlight that can be applied to different entries, you should enter an ASL expression in the text box, or compose the ASL expression in the *Atom Selection* dialog box, by clicking *Select*. For example, you could use atom sets or SMARTS patterns to define a particular functional group to highlight.

For silhouettes, you can choose the color and the transparency of the border in the Atoms tab. These values are stored separately for each silhouette highlight. You can change the width of the borders for all silhouettes in the Settings tab.

For contrast and saturation highlights, you can change the value of the contrast or the saturation in the Settings tab. These values are stored globally and apply to all highlights of the given type.

If you want to create a highlight quickly, with the current settings in the Manage Highlights panel, select a structural type from the Quick Highlight button menu, and pick atoms for the highlight in the Workspace.



If you already have a highlight that you want to modify for another purpose, select it in the table, and click Duplicate. A new row is added to the table with the duplicated highlight, and the row is selected. The name of the duplicate has a suffix, *-dupn*, appended to the name of the original. You can then start editing the duplicate to create a new highlight.

To edit any highlight, select it in the table. You can then change the name by editing the table cell, or change any of the settings that define the highlight in the Atoms tab (and the Text and Arrows tabs—see below).

To delete a highlight, select it in the table and click Delete.

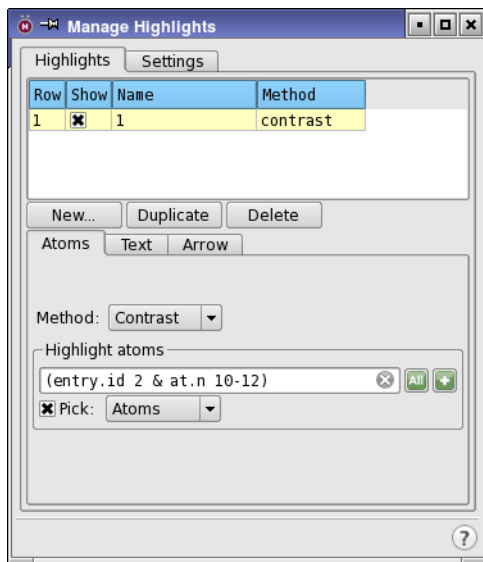


Figure 8.4. The Manage Highlights panel.

## 8.5.2 Adding Text and an Arrow to a Highlight

You can add text to the highlight in the Text tab. The text itself is entered in the text area, and is laid out exactly as you type it, with line breaks. The font type, size, and style can be chosen from option menus, and the color of the text can be chosen from a standard color selector, by clicking Edit. You can choose whether to have a transparent background, which means that anything that is behind the text will be visible through the text; or an opaque background, whose color is chosen automatically to contrast with the text.

Highlight text can be edited by double-clicking it in the Workspace, or right-clicking and choosing Edit. The Edit Highlight Text dialog box opens, in which you can change the text, background, and font. You can also edit it in the Manage Highlights panel, by choosing the highlight in the table, then editing the text in the Text tab.

If you want to delete highlight text, select the text in the Workspace and press Delete, or choose Highlight Text from the Delete button menu, or choose Delete Selected Highlight Text from the highlight text shortcut menu. You can select multiple text boxes to delete, with shift-click and control-click.

If you have defined some text, you can also add an arrow from the text box in the Workspace to a location relative to the structure, in the Arrow tab. To define the location of the arrow head, use the Arrow head centroid picking tools. The head is placed at the centroid of the picked atoms. The head of the arrow is defined as a point in 3D space, so it moves as you rotate or translate the structure. You can keep the arrow in the plane of the screen ( $xy$  plane) by selecting Flat in the General section of the Settings tab; selecting Pointing allows the arrow head to move in the  $z$  direction as well. The text does not move with the structure, but you can relocate it by dragging. If you want to move multiple text boxes simultaneously, you can select them with shift-click and control-click, and drag them.

When text is added to a highlight, you can choose whether to display the text only when there are atoms highlighted in the Workspace for this particular highlight, or it can be always shown when the highlight is selected for display. To make this choice, select or deselect Show only when atoms are highlighted. If this option is deselected, you can create a highlight consisting of text (and arrow) only, by not selecting atoms for the highlight.

## 8.5.3 Displaying Highlights

By default, when you create highlights, they are displayed in the Workspace. If you want to display or undisplay a highlight, you can click in the Show column of the highlights table. You can also choose to display the text (and arrow) for the highlight only when the Workspace contains atoms that match the ASL expression for the highlight, by selecting Show only when atoms are highlighted in the Text tab for the highlight.

## 8.6 Displaying Entry Properties

Properties for a single entry can be displayed in the Workspace if you have an entry included in the Workspace that is uniquely defined by a set of conditions. This entry is called the “target entry” and the conditions are:

- It is the only entry included in the Workspace
- It is the only entry included in the Workspace that is not fixed
- It is the only entry included in the Workspace that is selected

This display of properties for an entry is called *feedback*, or single-entry feedback. You can choose the properties that are displayed in the Preferences panel, under Feedback – Entry (see [Section 14.5.2 on page 354](#)).

Feedback can be displayed or hidden by any of the following methods.

- Choosing Workspace → Single Entry Feedback.
- Pressing the S key when the focus is in the Workspace.
- Selecting Show single-entry feedback in Workspace in the Preferences panel, under Feedback – Entry.
- Clicking the Feedback button on the Labels toolbar.



## 8.7 Other Objects

There are a few other objects that you can display in the Workspace, by choosing from the Workspace menu:

- Dipole Moment—Display the dipole moment of the structure as an arrow in the Workspace. If the structure has a dipole moment computed by a program (such as Jaguar), it is used for the display, otherwise the dipole moment is computed from the partial charges of the atoms (which can be Jaguar ESP charges if you calculated them). If no dipole moment appears, you can choose Tools → Assign Partial Charges to compute the partial charges from the OPLS\_2005 force field. The arrow can be configured in the Preferences panel—see [Section 14.4.7 on page 347](#).
- Coordinate Axes—Display a set of coordinate axes in the lower left corner of the Workspace. These axes show the orientation of the Workspace view, and rotate along with the structures when you perform a rotation.





# Projects

When you use Maestro, you are always working within a *project*. Projects are made up of *entries*, which can include multiple structures as well as properties of those structures. Project entries and their properties are displayed in the Project Table. You can perform a variety of operations on entries through the Project Table. By default, the Project Table panel is opened automatically when you open a project. You can change this behavior in the Preferences panel. To open the Project Table panel, choose Show Table from the Project menu, or click the Table button on the Project toolbar.



The project data is stored in a directory whose base name has the extension `.prj`. This directory is created in Maestro's current working directory. If you have not explicitly opened an existing project or created a new project, a scratch project is created in a temporary directory. You can specify this directory as a preference—see [Section 14.1.2 on page 332](#) for more information on setting the preference and the default location.

This chapter discusses in some detail how to use the Maestro Project Facility.

## 9.1 Project Operations

The Project menu of the main window enables you to perform operations on the project level. To perform operations on entries in the current project, use the menus in the Project Table panel. This section describes the operations that you can perform on projects.

### 9.1.1 Creating and Opening Projects

When you start Maestro without specifying a project to open, a scratch project is created. You can work with a scratch project, and perform nearly all the tasks that you can perform with a named project. If you want to start a new project and save its data, you can create a new named project by choosing Project → New. The main difference between a new project and a scratch project is that the new project has a name and is automatically saved. When you choose New, a project selector panel is displayed. This panel enables you to choose the location of the new project, create a directory, and type in the project name.

To open a recently used project, choose the project from the Project menu. To open any other project, choose Project → Open, or click the Open button on the Project toolbar.



A project selector panel is displayed that enables you to select a project to open. The project selector panels are described in more detail in [Section 9.1.7 on page 177](#). On Windows, you can open a project in a new Maestro session by double-clicking its icon.

You can only have one project open at any time.

If you are opening a project from a previous release, the project might have to be converted to the current release format. When you choose the project to open, the Convert Project dialog box opens. This dialog box allows you to specify a name for the converted project (as the original project is kept). Attempts at data extraction are made if errors occur during conversion.

In addition to opening projects (with extension `.prj`), you can also open zipped projects (with extension `.prj.zip` or `.prjzip`). These projects are uncompressed as temporary projects, and must be saved as named projects in order to be kept. To create a zipped project, simply zip the desired project directory, which has a `.prj` extension. You can open zipped projects directly from a web page—the `.prjzip` extension is registered when Maestro is installed on Windows; on Unix you have to register it.

### 9.1.2 Saving and Closing Projects

The data in a project is normally saved automatically when you make changes to the project. Changes to entries that are made in the Project Table are saved automatically. The saving of changes to entries that are displayed in the Workspace depends on the preferences you set in the Preferences panel. By default these changes are saved automatically.

Because the data in a named project is automatically saved you do not need to explicitly save the project. When you have finished working in a project you need only close the project, by choosing Close from the Project menu. If you want to work on a different project, you do not need to close the old project before opening the new project. When you close a project without opening a new project, a scratch project is created.

If you are working in a scratch project and decide you want to save it as a named project, or if you want to save a named project with a different name, choose Save As from the Project menu or click the Save As button on the Project toolbar.



A project selector panel is displayed that enables you to enter the name and choose the location of the project, and if necessary, create a directory. The panel is described in [Section 9.1.7 on page 177](#). If you choose **Close** when you are working in a scratch project, you are prompted to save the scratch project.

When a project is saved, all view transformations (translation, rotation, and zoom) are saved with it and restored when the project is opened. In addition, all user-defined sets of atoms are saved with the project and included when the project is copied or merged with another project.

If you want to make a copy of a project, you can do so in three ways, by choosing from the **Project** menu:

- **Save As**—A copy is made of the project, and the copy becomes the current project. This choice allows you to preserve the original project under its original name, and create a new project to work in.

Any jobs that you started in the original project are incorporated into the original, not the new project. However, if the project was a scratch project and you save it as a named project, jobs started from the scratch project are not incorporated. In that case, you must import the results manually into the named project.

- **Export Project**—A copy is made of the project, and the current project continues to be the current project. This choice allows you to make a backup of a project and continue to work in the same project. You can select options to copy user-created files that are in the project, to copy workflow data for Prime, Phase, and CombiGlide, to save the project in compressed, or zipped, form (`.prjzip`), and to save the project in Maestro 9.3 project format. You can also choose to copy only the selected or included entries into the copied project. Plots are only copied if you copy all entries.
- **Publish**—Create a web page (`.htm` or `.html`) that contains a relative link to a compressed copy of the project. You can provide a summary of the project, which is included in the web page. Because the link is a relative link, you can copy the page and the project to a suitable location for access on your web site, or copy the link from the page to a suitable page on your web site.

You can also copy a project with the UNIX `cp -r` command. A project is simply a directory with various files stored in it for the administration of the project.

### 9.1.3 Backing Up Projects

In addition to saving a copy of a project, you can make backups of projects to guard against data loss. To do so, choose **Project** → **Back Up**. The **Project Backup Description** dialog box opens, in which you can enter a short description of the backup. This description can be used to identify the backup if a project has to be restored from backup. When you click **OK**, the backup

commences. The backup is stored in zip format, named with the time stamp as `YYYY.MM.DD-HH.MM.SS.prj.zip`. The backups for a project are written to the directory `project.backup`, which is created in the same directory as `project.prj`. The backups are therefore outside the project itself, but in the same location as the project. You can specify an alternate location in the Preferences panel—see [Section 14.2.2 on page 337](#).

You can schedule automatic backups of projects, by making settings in the Preferences panel—see [Section 14.2.2 on page 337](#). You can also set preferences for the number of backups to keep, and whether to issue a notification when the backup finishes.

To revert to a saved backup, choose **Restore from Backup** from the Project menu. The **Restore Project from Backup** dialog box opens, and presents a table of backups with the backup time and description listed. Select the backup you want to restore, and click **OK**. The backup that you restore overwrites the current project, so if you want to keep data from the current project you should export it first.

You can also save the state of a project, which is a compressed copy of the project that is stored inside the project directory. This is useful when you want to make changes that you might want to revert later. To save the state, choose **Project → Save State**; to revert to this state, choose **Project → Revert to Saved State**.

### 9.1.4 Recovering Projects

If a project is corrupted for some reason, Maestro tries to recover the data from the project when it is opened. First, a warning dialog box is posted, indicating that Maestro cannot open the project. When you click **OK**, the **Recover Project** dialog box opens. This dialog box offers up to three options for project recovery

- **Recover using the opening state**—If the project had a compressed opening state, use this to recover the project. Any information added to the project after it was last opened is lost. This option is not available if the project did not have a compressed opening state. The option applies to projects created from Maestro 9.7 or earlier.
- **Recover using a previously generated backup**—Use a zipped backup of the project to recover the project. Any information added to the project after the backup was made is lost. If you have made multiple backups, a dialog box is displayed, in which you can choose the backup. See [Section 9.1.3](#) for information on backing up projects.
- **Recover usable pieces**—Recover as much data from the corrupted project as possible. This option uses the utility `project_extract`, which is described in [Section D.4 on page 435](#).

The corrupted project is renamed from `project.prj` to `project-corrupted.prj`, and the recovered version is named `project.prj`.

## 9.1.5 Deleting Projects

If you do not want to keep the current project you can remove it by choosing **Delete** from the **Project** menu. You will be prompted to confirm the deletion of the project. When you delete a project, any jobs associated with that project are killed and purged from the job database.

You can also delete the project from a terminal window by entering the command

```
rm -rf project_name
```

When you delete a project using `rm`, job files that were created using the project are not deleted unless they are located within the project directory.

## 9.1.6 Undoing Project Operations

Changes made directly to the Project Table are saved immediately, regardless of your synchronization preference. This preference affects only the changes made in the Workspace. (For information on synchronization preferences, see [Section 14.2.3 on page 339](#).) Some of these changes can be undone with **Edit** → **Undo**, but you can only undo the last change made.

You can save the state of your project before performing operations that you might want to undo. To save the state of the current project, choose **Project** → **Save State**. If the synchronization mode you have selected is **When approved by user**, and you have modified entry structures in the Workspace but have not synchronized the changes, you are prompted to do so.

To revert to the saved state, choose **Project** → **Revert to Saved State**.

## 9.1.7 The Project Selector Panels

Many of the project operations—creating, opening, saving—involve selection of a project location on disk. Each of these operations has a project selector panel. The project selector panels are file selectors that are configured so that Maestro project directories (those with `.prj` extensions) or zipped projects (those with `.prjzip` or `.prj.zip` extensions) are the only visible items. These items appear in the current directory listing with a project icon.



File selectors are described in detail in [Section 1.1.4 on page 3](#).

Only one instance of a given project can be open at a time. A project is locked if you or someone else already has the project open. To indicate whether a project is in use, a lock icon is placed on the icon for each locked project.



When you merge projects you can choose to include any user-created files by selecting Include User Created Files.

If you are creating a new project, you do not need to add the `.prj` extension, which Maestro supplies if it is absent.

### 9.1.8 The Project Summary Panel

Projects can be large, diverse collections of data. To help you keep track of the project, Maestro provides a Project Summary panel. This panel displays information about the current project, including annotation of the project, information on jobs run from the project, and information on runs saved from wizard-based panels. To open this panel, choose Summary from the Project menu. The panel has three sections: Annotation, Project, and Jobs.

**Annotation section:** This section displays the project annotation. Because projects are frequently modified, it may be helpful to annotate your project. The project creation date and job history are automatically added to the project annotation.

You can edit the text in the annotation section, including the automatically generated text. The standard mouse actions (highlight to copy, middle-click to paste) can be used to copy and paste text. The main key strokes for editing text are:

- CTRL+W to cut the selection
- ALT+W to copy the selection
- CTRL+Y to paste the selection

These and other conventions are the same as those used by the Emacs editor. For more information, visit the web site <http://www.tcl.tk/man/tcl8.4/TkCmd/text.htm#M152>.

**Project section:** This section displays statistics on the project, in two subsections, Entries and Runs. The Entries subsection has a button to open the Project Table panel. The Runs subsection displays information on jobs run for various products and has buttons to open product panels.

**Jobs section:** This section displays the jobs in the job database for the current project. Clicking Refresh updates the display for all jobs, and is equivalent to clicking Monitor in the Monitor panel. Clicking Delete deletes the selected jobs from the database. You can select jobs with the usual click, shift-click and control-click key strokes.

## 9.2 Adding Entries to a Project

Projects are made up of entries. Entries can contain multiple structures and their properties. Each entry has an entry ID, an entry name, and a title.

- The entry ID is used to identify entries internally and is guaranteed to be unique. It is also used to select entries. It is assigned by Maestro and is noneditable.
- The entry name can be used to identify entries in ASL expressions. It is guaranteed to exist, and is assigned by Maestro if it does not exist, but is not guaranteed to be unique. Entry names can be edited.
- The title can be set or changed by the user but is otherwise not modified by Maestro. The title is displayed in the Project Table by default, but the entry name is not.

Entries can be grouped into *entry groups* for convenience. Each entry group has a title.

You can add entries to a project by importing structures from a file, by creating entries from structures you have built in the Workspace, or by merging entries from a different project. In addition, you can create new entries by splitting or duplicating an existing entry, or by incorporating the results of a job into the project.

### 9.2.1 Importing Structures From a File

When Maestro imports structures from a file, the structures are copied, translated into entries, and incorporated into the current project. Structures can be imported from Maestro, Macro-Model, PDB, Mol2, SD, and other files using the Import panel. Multiple molecular structures can be imported simultaneously from multiple files, and you can choose which structures, if any, are included in the Workspace upon import. Entry names and titles are automatically assigned if they do not exist, and are read if they do exist. See [Section 3.1 on page 41](#) for more information on importing structures.

### 9.2.2 Creating Entries From Workspace Structures

To save a scratch entry as a project entry—or to create a new entry from existing entries in the Workspace—choose **Create Project Entry** from the Workspace menu or from the selection shortcut menu, type CTRL+SHIFT+N (⇧⌘N), or use the **Create Entry** button on the Workspace toolbar.



The Create Project Entry dialog box opens, in which you can type an entry title, and choose whether to create the entry from the selected atoms, the displayed atoms, or all atoms in the Workspace.

If all the atoms in the new entry come from a single entry group, the new entry is placed in the same group. Otherwise, it is added to the end of the ungrouped entries.

A scratch entry is created, for example, when you draw a structure with the Draw tool.

### 9.2.3 Pasting Structures Into the Workspace

You can paste structures into the Workspace from another application, provided they were copied to the clipboard in SMILES or MDL format. A new entry is created for these structures. For example, on Windows you can paste structures from ChemDraw and Isis Draw. See [Section 3.7 on page 61](#) for details.

### 9.2.4 Incorporating Entries From Job Output

When you use selected or included entries from a project as input for most kinds of jobs, you have the option to incorporate the job results as entries in the Project Table. You can choose to append the new entries, to replace the input entries with the new entries, or you can choose to ignore the output and not incorporate them into the table at all.

If the job results contain multiple structures, by default an entry group is created for them on incorporation if one does not exist, with the group title set to the name of the file from which the entries were incorporated, minus the extension. You can choose to append the entries individually rather than as a group when you run the job from Maestro. See [Section on page 194](#) for more information on entry groups.

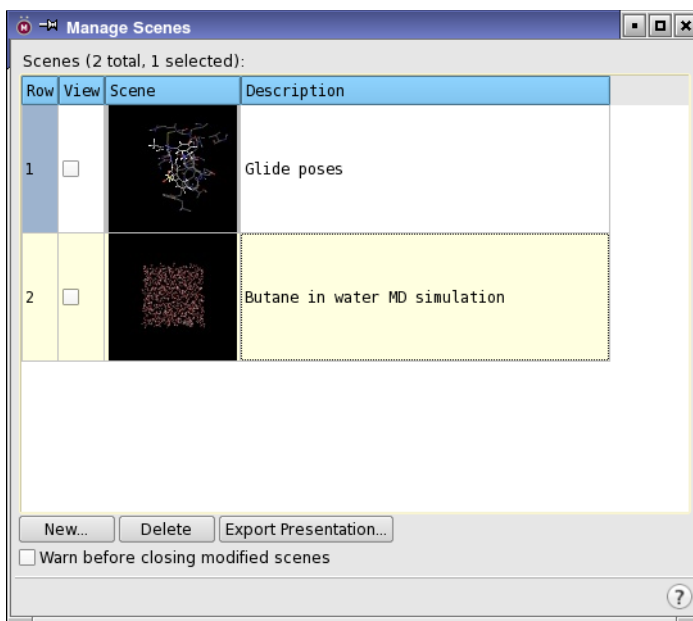
For more information on incorporating job output into the project, see [Section 2.9](#) of the *Job Control Guide*.

### 9.2.5 Merging Entries From Another Project

You can merge the entries from a specified project into the current project. There is no facility for merging a subset of entries. When the merge is performed, the entries are incorporated at the end of the Project Table list in the current project, and are selected. Any conflicts between group titles are resolved by adding a numerical suffix to the incoming group titles.

To copy the entries from a source project into the currently open project, choose **Merge** from the Project menu. In the Merge From Project project selector, navigate to the desired source project. If you want to include user-created files associated with the merge source project, select **Include user created files**.





**Figure 9.1.** The Manage Scenes panel.

## 9.3 Using Scenes

Maestro provides a way of storing multiple “snapshots” of a project or a subset of a project, called *scenes*. Scenes are stored as mini-projects inside the main project, in zipped format (.prj.zip). Scenes include a set of entries, with associated data, and all aspects of the Workspace state, such as the entries included, display options, measurements, and so on, so that you can display the scene exactly as it was when you saved it. However, scenes do not include scratch entries. Scenes do not include plots, job information, or run data from CombiGlide, Prime, or Phase. They do not include information on panel layout or which panels are open, or which components are visible in the main window.

Scenes can be managed from the Manage Scenes panel, which you open by choosing Workspace → Scenes → Manage.

To create a new scene, choose Workspace → Scenes → New, click New in the Manage Scenes panel, or click the New Scene button on the Workspace toolbar.

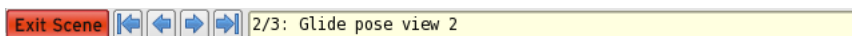


If there is a scratch entry in the Workspace, you are prompted to save it as a project entry; if you do not, it is discarded. The New Scene dialog box opens, in which you can provide a text description of the scene, and choose which project entries to include in the scene. Once a scene is saved, it is listed in the Scenes table of the Manage Scenes panel. The table row for the scene includes a numerical index for the scene, a button to view the scene, a fingernail image of the Workspace, and the description that you provided. You can edit the description by double-clicking in the table cell. To reorder the rows, select them and drag them to the new location in the table.

To delete scenes, select them in the table and click Delete or choose Delete from the shortcut menu.

Because scenes are part of a project, you can display them without closing the current project. When you display a scene, it behaves like a regular project. You can work within the scene just as in a project, making changes and running jobs. The Maestro panels have access only to the entries in the scene. Any changes you make are not saved by default, however. If you want to save changes, select Warn before closing modified scenes. When you close a scene that has changed, a dialog box is displayed in which you can replace the scene with the modified scene (Replace), discard the changes and keep the original scene (Discard), or return to the scene (Cancel). If this option is not selected, you can right-click in the scene row and choose Replace. save the modified scene as a new scene and delete the original scene. You can also create a new scene from the displayed scene, just as you can from a project.

To display a scene, click the View column in the Scenes table of the Manage Scenes panel. The scene is recalled and the Workspace structure is displayed as it was when the scene was saved. The Scenes toolbar is displayed below the Workspace. This toolbar is a visual indication that you are working in a scene, not the parent project.



The toolbar allows you to quickly step between scenes, by using the arrow buttons. You can also use the UP ARROW and DOWN ARROW keys in the Manage Scenes panel to change scenes. This is useful if you store a set of scenes that show different stages or aspects of a project and want to use these scenes as a presentation. The scene changes are animated using the preferences set in the Workspace tab of the Preferences panel. You can also use the toolbar to exit the scene and return to the project. Only one scene can be displayed at a time. The toolbar can also be displayed by choosing Workspace → Scenes → View, or clicking the View Scenes button on the Workspace toolbar.



You can create a presentation from a set of scenes that contains only the scenes. The presentation is stored as a project that contains only the scenes. If you store it in zipped format (the default), you can easily transfer it or send it by e-mail. To do so, click **Export Presentation** in the **Manage Scenes** panel. The **Save Project** panel opens, in which you can navigate to a location and save the presentation. Because the scenes are read-only, you can make changes when you show the presentation to others, and be assured that the presentation itself is not changed.

You can export the current scene as a project, by choosing **Export as Project** from the shortcut menu. A file selector opens so that you can navigate to a location and name the project.

## 9.4 The Project Table Panel

The **Project Table** panel provides access to a range of tools for managing the data in the project and operating on that data. The panel contains a menu bar, several toolbars, the **Project Table** itself, and a status bar. This section provides a brief description of the basic table operations, the tools, and the use of the mouse and shortcut keys for performing various operations.

Each project entry is represented by a row in the **Project Table**. Three columns of the **Project Table** are always visible: the row number, the **In** column, which has an icon indicating whether the entry is displayed in the **Workspace**, and the **Title** column, which contains buttons for auxiliary data as well as the title. The buttons are for display of Phase hypotheses (H), surfaces (S), trajectories (T), and vibrational frequencies (V). The **Stars** column can be hidden. The remainder of the columns appear in the scrolling section of the table, including the entry name and the entry ID. The entry name can be displayed or undisplayed from the **Property** menu.

Project entries have two states that represent how they are being used: the *selection* state and the *inclusion* state. Selected entries are highlighted in the **Project Table** and are available for

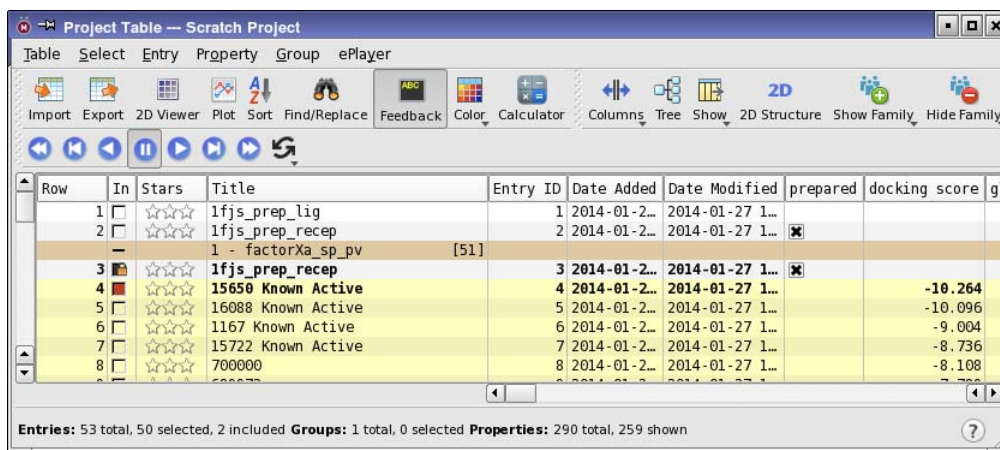


Figure 9.2. The **Project Table** panel.

operations such as copying, deleting, or use as input to a computational program. Selection of entries is discussed in the next section. Included entries are displayed in the Workspace, and are available for manipulation, modification, and other actions that can be performed from the Workspace. The selection and inclusion states are stored in the project, so they are restored when you reopen the project.

The inclusion state is indicated in the In column. Excluded entries—entries that are not displayed in the Workspace—are marked with an empty square. Included entries are marked with a filled square. Fixed entries—entries whose display is not affected by the inclusion or exclusion of other entries—are marked with a padlock icon. Fixed entries are not frozen: you can perform operations on fixed entries in the Workspace, such as rotation and translation, or adding or deleting atoms. To undisplay a fixed entry, you must exclude it from the Workspace. The marker for an included entry is red for the *target* entry—a single entry for which information can be displayed in the Workspace and which can be marked.

### 9.4.1 The Project Table Toolbars

There are four action toolbars: Project, Property, Find, and ePlayer, and in addition a Manager toolbar that you can use to show or hide the toolbars. You can show or hide the toolbars by choosing Table → Toolbars → *toolbar*. The Find toolbar and ePlayer toolbar are described in later sections ([Section 9.4.9 on page 196](#) and [Section 9.7 on page 216](#)). This section describes the Project and Property toolbars.

You can select the buttons that are shown on the toolbars by choosing Table → Customize → Toolbars or by right-clicking in a toolbar and choosing Customize.

#### 9.4.1.1 Project Toolbar

The buttons on the Project toolbar are described briefly below. The use of these buttons is discussed in other sections.



##### Import

Import structures into the Project Table as new entries. Opens the Import panel. See [Section 3.1 on page 41](#).



##### Export

Export structures from the Project Table to file. Opens the Export dialog box. See [Section 3.2 on page 52](#).



##### 2D Viewer

Display 2D structures in a grid. Opens the 2D Viewer panel. See [Section 9.9.2 on page 220](#).



##### Plot

Plot property values for the selected entries. Opens the Manage Plots panel. See [Chapter 11](#).

**Sort**

Sort entries or entry groups, with optional group assignment and entry selection. Opens the Sort Project Table panel. See [Section 9.6.12 on page 211](#).

You can sort by a single property from the shortcut menu for the property column header.

**Find/Replace**

Find and replace alphanumeric text in any column of the Project Table except for the row number. Opens the Find panel. See [Section 9.4.9 on page 196](#).

**Feedback**

Display information about a single entry, termed the “target” entry, in the top left corner of the Workspace. See [Section 8.6 on page 171](#).

**Color**

Color the rows in the Project Table for the selected entries. See [Section on page 194](#) and [Section 9.11.13 on page 242](#)

**Calculator**

Perform calculations by combining properties of project entries. Opens the Project Table Calculator panel. See [Section 9.11.3.4 on page 230](#).

### 9.4.1.2 Property Toolbar

A description of the buttons on the Property toolbar is provided below. The use of these buttons is discussed in other sections.

**Columns**

Resize columns. Displays a menu from which you can choose an option for adjusting the column widths. See [Section on page 194](#).

**Tree**

Display a tree view of the properties in the Project Table. Opens the Property Tree panel, which is docked to the right of the properties in the table. See [Section 9.11.11 on page 237](#).

**Show**

Show properties in the Project Table. See [Section 9.9.2 on page 220](#).

**2D Structure**

Display 2D structures in the Project Table as the third or fourth column, labeled 2D Structure. See [Section 9.9.1 on page 220](#).

**Show Family**

Show only properties from the selected property family. Choose the family from the menu. See [Section 3.1 on page 41](#).

**Hide Family**

Hide properties that are from the selected property family. Choose the family from the menu. See [Section 3.2 on page 52](#).

## 9.4.2 The Project Table Menus

The menus on the Project Table menu bar are described briefly below. The use of the menu items is discussed later in this chapter.

- **Table**—find text, sort entries, plot properties, import and export structures and data, perform calculations on properties, and configure the Project Table.
- **Select**—select all entries, none, invert your selection, make a random selection, or select classes of entries using the Entry Selection dialog box and the Filter panel.
- **Entry**—include or exclude entries from the Workspace, perform various operations on the selected entries, group or ungroup entries, enter Pose Viewer mode.
- **Property**—display and manipulate entry properties in the Project Table.
- **Group**—select, display, and delete entry groups.
- **ePlayer**—view entries in succession, stop, reverse and set the ePlayer options.

## 9.4.3 The Project Status Bar

The status bar, located at the bottom of the panel, shows information about the project entries: total number, number selected, and number included. It also shows information on the number of groups and selected groups, and the number of properties in total and shown.

When the pointer is over a toolbar button, the display is replaced by information about that button.

## 9.4.4 Mouse Functions in the Project Table

The standard use of shift-click and control-click to select objects is supported in the Project Table. Middle-click is supported as an alternative to control-click. This behavior applies to selection of entries and inclusion of entries in the Workspace. Dragging to resize columns and to move rows is also supported. You can drag a set of non-contiguous entries to reposition them in the Project Table—see [Section 9.6.11 on page 210](#) for more information. You can edit cells by clicking in the cell and changing the text, then pressing ENTER or clicking elsewhere in the Project Table. You can scroll vertically through the Project Table using the scroll wheel.

A summary of project-based mouse functions is provided in [Table 9.1](#).

Table 9.1. Mouse operations in the Project Table.

Task	Mouse Operation
Change a Boolean property value.	Click repeatedly in a cell to cycle through the possible values (On, Off, Clear).
Display the Entry menu for an entry.	Right-click anywhere in the entry. If the entry is not selected, it becomes the selected entry. The chosen action is applied to all selected entries.
Display a version of the Property menu for a property.	Right-click in the column header.
Edit the text or the value in a table cell.	Click in the cell and edit the text or value. If the entry containing the cell is not selected, it is selected. The cursor is placed at the end of the data by default, and the data is selected.
Include an entry, exclude all others.	Click the In column of the entry.
Move selected entries.	Drag the entries.
Paste text into a table cell.	Middle-click.
Resize columns.	Drag the boundary.
Select an entry, deselect all others.	For an unselected entry, click anywhere in the row except the In column; for a selected entry, click the row number.
Select or include multiple entries.	Click the first entry then shift-click the last entry.
Toggle the entry selection or inclusion state.	Control-click or middle-click the entry or the In column.
Scroll through the entries	Use the wheel to scroll one entry at a time; hold down SHIFT and use the wheel to scroll a page at a time.

### 9.4.5 Project Table Shortcut Menus

In addition to the menus on the menu bar, the Project Table panel has shortcut menus, which are displayed when you right-click and hold in the table. There are three main shortcut menus: one for properties, one for entries, and one for entry groups.

- **Property shortcut menu:** This menu duplicates some items on the Property menu, and has some additional items. It is displayed when you right-click and hold over a column header, and the actions are applied to the property in the column. The items on this menu are described in [Table 9.2](#).

Table 9.2. Property shortcut menu items.

Menu item	Action
Hide	Hide (undisplay) the property. Also available in the Entry List panel.
Sort Selected Sort All	Sort the table rows by the values of the property. There are four items, for sorting the selected rows or all rows, and in ascending (A-Z) or descending (Z-A) order. Also available in the Entry List panel.
Fit To	Fit the column width to the width of the data, the header, or the larger of the two. The choice is made on the submenu (Header, Data, Header+Data). Also available in the Entry List panel.
Move To	Move column to another location. The submenu contains First, Before, Left, Right, After, and Last, for moving columns within the scrolling area, and Fixed Area and Scrolling Area, for moving columns between the fixed and scrolling areas. Properties moved to the fixed area are placed at the end of the fixed area.
Reorder	Reorder some or all properties. Opens the Reorder Properties dialog box, in which you can select the properties to move and their new location.
Edit Name/ Type	Change property names. Opens the Edit Property Name/Type panel, in which you can edit the visible name or the internal name of any property except those whose names are reserved.
Decimal Places	Set the decimal precision of real properties. Opens the Set Decimal Places dialog box, in which you can select properties, set the precision, and apply E notation. This item is present only if the column contains a real-valued property.
Change Case	Change the case of a string-valued property. The submenu offers the choice of lower-case (change all values to lower case), UPPERCASE (change all values to upper case), and Title Case (change first letter of each word to upper, rest to lower case). This item is present only if the property is a string property and changes are permitted. You cannot change the case of these properties: Entry ID, Date Added, Date Modified, PDB format version, original cms file, source file, Job Name, ct type.
Copy	Copy values from one property to another. Opens the Copy Property panel, in which you can specify the target and destination property. Properties can be copied for the selected entries or for all entries.
Clear Values	Clear the values for the selected property.
Delete	Delete the selected property.
Workspace Feedback	Add or remove the property from the Workspace feedback. The submenu offers the choice of Add (add this property to the feedback), Replace (replace the feedback with this property), and Remove (remove this property from the feedback). Also available in the Entry List panel.



- **Entry shortcut menu:** This menu duplicates the Entry menu, except for Mark Target Entry and View Poses, and in addition has an Export submenu, which duplicates the Export submenu on the Table menu. It is displayed when you right-click and hold over any entry in the table. If the entry is part of the selection, the menu is displayed immediately. If the entry is not part of the selection, the entry is selected and all others deselected before the menu is displayed. The items on this menu are described in [Table 9.3](#).

Table 9.3. Entry shortcut menu items.

Menu item	Action
Include Only	Include only the selected entries in the Workspace, and exclude all others that are not fixed.
Include	Include the selected entries in the Workspace, without affecting the inclusion of others.
Exclude	Exclude the selected entries from the Workspace.
Fix	Fix the selected entries in the Workspace. Fixed entries must be explicitly excluded from the Workspace: they cannot be excluded by inclusion of other entries.
Unfix	Change the inclusion status of fixed entries so that they are included but not fixed. The padlock icon is removed from the In column for these entries.
Lock	Lock entries so that they cannot be changed or deleted. A padlock icon is displayed next to the row number.
Unlock	Unlock entries so that they can be changed or deleted.
Stars	Set the number of stars in the Stars property.
Delete	Delete the selected entries, without confirmation. If you deleted entries unintentionally, click the Undo button on the main toolbar.
Merge	Merge the selected entries into a single entry. The name of the new entry is merge, and the title is the title of the first selected entry. The new entry goes immediately after the last selected entry.
Duplicate	Duplicate the selected entries, and select the duplicates. Submenu with four actions: In Place—place each duplicate after its original in the table. Ungrouped—move the duplicates out of the group that the originals were in, if applicable. Entries that were moved out of a group appear at the end of the ungrouped entries; entries that were not grouped appear after their parents. Into New Group—move the duplicates to a new entry group. A dialog box opens so you can name the group. Into Existing Group—move the duplicates into an existing group. A dialog box opens so you can select the group.

Table 9.3. Entry shortcut menu items. (Continued)

Menu item	Action
Split	<p>Split the selected entry into a set of entries. The source entry is not changed. The new entries inherit the title of the source entry. Submenu with three actions:</p> <p><b>By Molecule</b>—create one entry for each non-water molecule, and one for all water molecules. The entries are named by appending <code>_moln</code> to the entry name of the source entry, where <i>n</i> is an integer starting from 1.</p> <p><b>By Chain</b>—create one entry for each chain and one for all water molecules. The entries are named by appending the chain name to the source entry name. A Chain Name property is added to the entries to store the chain name.</p> <p><b>Into Ligands, Water, Other</b>—create one entry for each ligand-sized molecule, one for all water molecules, and one for all other atoms, such as receptor and cofactors.</p> <p>You can also set an option to copy properties to the new entries.</p>
Copy Properties	Copy the properties from the selected entry onto the clipboard, for pasting into one or more entries. The submenu offers the choice of <b>All</b> , to copy all properties, or <b>Shown</b> , to copy only the displayed properties.
Paste Properties	Paste properties from the clipboard into the selected entries. The copied properties overwrite any existing properties of the same (internal) name. If a property does not exist (or is of a different type) a new property is created and values are added for the selected entries. If a property value is blank (null) in the copied property, it still overwrites values in the target entries.
Move to Row	Move the selected entries in the table to start at a given row number. Opens a dialog box in which you can specify the row number, or choose <b>First</b> or <b>Last</b> .
Group	<p>Perform grouping operations on the selected entries. Submenu with four actions:</p> <p><b>New</b>—Create an entry group from the selected entries. A dialog box is displayed, in which you can enter the title of the group.</p> <p><b>Move To</b>—Move the selected entries to a chosen group. A dialog box opens, in which you can select an existing group, no group, or create a new group.</p> <p><b>By Entry Property</b>—Create entry groups based on the properties of the entry. Opens the <b>Group by Entry Property</b> panel, in which you can name the groups, select the property, set conditions on the property, and create the groups.</p> <p><b>Ungroup</b>—Move the selected entries out of the group they are in. The entries are placed at the end of the ungrouped entries.</p>
Color	<p>Color the rows in the Project Table for the selected entries. Submenu with three actions:</p> <p><b>Constant Color</b>—Color the rows for the selected entries with a chosen color. Opens a color selector so you can choose the color.</p> <p><b>By Entry Property</b>—Color the cells for a given property by the value of the property. Opens the <b>Color by Property</b> dialog box.</p> <p><b>Reset Colors</b>—Reset the row colors of the selected entries to the defaults.</p>

Table 9.3. Entry shortcut menu items. (Continued)

Menu item	Action
Export	Export the selected entries. Submenu with three actions: Structures—Export structures and properties. Opens the Export dialog box. Spreadsheet—Export properties in CSV format. Opens the Export Spreadsheet panel. To Canvas—Export structures and properties to Canvas. Opens Canvas with the structures imported into a new Canvas project.

- **Entry group shortcut menu:** This menu includes the Collapse and Expand items that are on the Groups menu and a number of other items. It is displayed when you right-click and hold over an entry group row. The items on this menu are described in [Table 9.4](#). There are four groups of items: for entry selection, for entry inclusion, for group management, and for actions on group members.

Table 9.4. Entry group shortcut menu items.

Menu item	Action
Edit Title	Edit the title of the group. Only displayed when the pointer is in the Title column. Not available in the Entry List panel (see <a href="#">Section 9.10 on page 223</a> ).
Duplicate	Duplicate the group. The duplicate group is placed below the source group. Duplication makes copies of all the entries in the source group and places the copies in the new group.
Ungroup	Move the entries out of the group, and delete the group. The entries are placed at the end of the ungrouped entries.
Delete	Delete the group, and all the entries in it. A confirmation dialog is displayed when you choose this item.
Include All	Include the entries in the group in the Workspace (with other included entries).
Include Only All	Include in the Workspace only the entries in the group, and exclude all others. Does not affect fixed entries.
Include First	Include the first entry in the group in the Workspace (with other included entries).
Exclude All	Exclude the entries in the group from the Workspace.
Collapse or Expand	Show or hide grouped entries. If the entries in the selected groups are visible, this item is Collapse, and the entries are hidden (the groups are collapsed). If the entries are not visible, this item is Expand, and the entries are shown (the groups are expanded). Each item has a submenu from which you can choose to collapse or expand all groups (All), or only the selected groups (Selected). The Expand submenu also has the item Only Selected, which allows you to expand only the selected groups and collapse all the others.

Table 9.4. Entry group shortcut menu items. (Continued)

Menu item	Action
ePlay	Play through the entries in the group with the ePlayer.
View Poses	Submenu that allows you to set up an entry group to display poses of a set of ligands in the context of a receptor, and calculate and display H-bonds and contacts for the poses.
Export Structures	Export the structures in the group. Opens the Export dialog box.

In addition to these shortcut menus, there are Surfaces and Hypotheses shortcut menus, which are displayed when you right-click an S button or an H button in the Title column. The Surfaces shortcut menu has two items, Hide All Surfaces, which undisplay all surfaces, and Display, which is a submenu with choices for the object to display: Surfaces Only, Structure Only, and Both. The Hypotheses shortcut menu provides tools for display of Phase hypotheses. This shortcut menu is described in detail in [Chapter 8](#) of the *Phase User Manual*.

### 9.4.6 Use of the Keyboard in the Project Table

Some frequently used operations have been assigned shortcut key combinations. The shortcuts, their functions, and their menu equivalents are listed in [Table 9.5](#).

Table 9.5. Shortcut keys in the Project Table.

Keys	Action	Equivalent Menu Choices
CTRL+A (⌘A)	Select all entries	Select → All
CTRL+D (⌘D)	Duplicate entry in place	Entry → Duplicate → In Place
CTRL+F (⌘F)	Find/Replace text	Table → Find
CTRL+I (⌘I)	Open Import panel	Table → Import Structures
CTRL+N (⌘N)	Include only selected entries	Entry → Include Only
CTRL+U (⌘U)	Deselect all entries	Select → None
CTRL+X (⌘X)	Exclude selected entries	Entry → Exclude
CTRL+Z (⌘Z)	Undo/Redo last command	Edit → Undo/Redo in main window

If you have Num Lock, Caps Lock, or Scroll Lock enabled, the shortcut keys do not work.

In addition to these shortcut keys that can be used in the Project Table, there is a range of keys that can be used both in the Project Table and the Workspace for project navigation and opera-

tions. These keys are summarized in [Table 9.6](#)

*Table 9.6. Project Table navigation and operation keys*

<b>Key</b>	<b>Description</b>
UP ARROW	Scroll the Project Table up one row.
DOWN ARROW	Scroll the Project Table down one row.
RIGHT ARROW	For each included entry, replace that entry in the Workspace with the next selected entry in the Project Table.
LEFT ARROW	For each included entry, replace that entry in the Workspace with the previous selected entry in the Project Table.
HOME	Scroll the Project Table to the top.
END	Scroll the Project Table to the bottom.
PAGE UP	Scroll the Project Table up one page.
PAGE DOWN	Scroll the Project Table down one page.
SHIFT+PAGE UP	Scroll the Project Table up to the previous selected entry, expanding groups as necessary.
SHIFT+PAGE DOWN	Scroll the Project Table down to the next selected entry, expanding groups as necessary.
CTRL+PAGE UP	Scroll the Project Table up to the previous included entry, expanding groups as necessary.
CTRL+PAGE DOWN	Scroll the Project Table down to the next included entry, expanding groups as necessary.
SHIFT+UP ARROW	Scroll the Project Table up by one group.
SHIFT+DOWN ARROW	Scroll the Project Table down by one group.
CTRL+UP ARROW	Scroll the Project Table up by one group, expand the group and collapse all other groups.
CTRL+DOWN ARROW	Scroll the Project Table down by one group, expand the group and collapse all other groups.
CTRL+SHIFT+UP ARROW	Scroll the Project Table up by one group; expand the group and collapse all other groups; and change the selection to only the entries in the expanded group.
CTRL+SHIFT+DOWN ARROW	Scroll the Project Table down by one group; expand the group and collapse all other groups; and change the selection to only the entries in the expanded group.
SHIFT+LEFT ARROW	Include only the first selected entry in the next entry group.

Table 9.6. Project Table navigation and operation keys (Continued)

Key	Description
SHIFT+RIGHT ARROW	Include only the first selected entry in the previous entry group.
CTRL+LEFT ARROW	Include the first selected entry (ePlayer Go to Start)
CTRL+RIGHT ARROW	Include last selected entry (ePlayer Go to End)
X	Mark or clear mark for the current entry. If the Mark property does not exist, create it and set the value for the entry to <code>true</code> (marked).
S	Display or undisplay entry information in the Workspace. This option is subject to a preference for display of single-entry feedback.

### 9.4.7 Configuring the Project Table

The Project Table panel provides tools for controlling what is displayed in the table. Some of these tools are also discussed later in this chapter. Many configuration options are available in the Preferences panel—see [Section 14.3 on page 341](#).

**Grouping and ungrouping entries.** You can group the selected entries by choosing Group from the Entry menu. A new entry group is created at the end of the table, and the entries are moved to the new location. You can display or hide the members of the group by clicking the In column for the group.

To ungroup an entry group, select the group and choose Ungroup from the Entry menu. The group entries are placed at the end of the ungrouped entries, immediately above the first group.

You can add the selected entries to an existing group by choosing Move to Group from the Entry menu, and selecting the group in the dialog box that is displayed. You can move entries out of a group by selecting them and choosing Move to Row from the Entry menu.

**Displaying or hiding properties.** You can display a subset of properties by choosing Property → Show → Select, then using the Show Property dialog box to select the properties to show or hide. You can choose individual properties or a family of properties. Property families are the properties generated by an application, such as QikProp, and are classified into primary and secondary properties. You can restrict the display to a property family directly, by choosing the family from the Show Only Family submenu of the Property menu. If you want to see only those properties that have values for the selected entries, choose Property → Show → For Selected Entries. See [Section 9.11.11 on page 237](#) for more information. You can hide all properties by choosing Property → Show → None.

**Displaying 2D structures.** You can display 2D structures in the Project Table as the third or fourth column, labeled 2D Structure. To do so, click the 2D structures toolbar button, or choose Property → Show → Show 2D Structures. The size of the structures can be controlled by changing the row height, which you do by dragging the row margin in the Row column. The structures displayed are images that are generated when they are displayed. You can set preferences for the maximum structure size and for image generation in the 2D Structures tab of the Preferences panel—see [Section 14.10 on page 364](#).

**Coloring by property values.** You can color the cells of the Project Table by the values of the properties in the cells. To do so, choose Color by Entry Property from the Entry menu, and make settings in the Color By Property dialog box. See [Section 9.11.13 on page 242](#) for more information.

**Coloring entries.** You can color the selected rows in the Project Table by choosing items from the Color submenu of the Entry menu or from the Color toolbar button. To apply a constant color, choose Constant Color and select the color in the color chooser that opens. To color rows by a property value, choose By Property Value, and make settings in the Color by Property dialog box. See for more information. The color is stored in the project for the colored entries. The property color and the selection color take precedence over the row color, but the row color is always shown in the first column (Row). To reset the color to the default color for the selected rows, choose Reset Colors.

**Resizing columns.** You can resize columns by dragging the border of the column. You can set the width of the columns to the width of the widest data item (Fit to Data), the width of the widest of the data and the heading (Fit to Header + Data), the width of the heading (Fit to Header), or to a fixed width (Fixed Width), by choosing from the Columns button menu on the toolbar, the Columns submenu of the Table menu, or the Adjust Width submenu of the Property shortcut menu. The “fixed width” is 2 characters for Boolean properties, and a maximum of 8 characters for other properties. If you double-click the right border of the column it fits the width to the column data.

**Aligning column data.** You can align the data in a column on the left boundary, the right boundary, or the center of the column, by right-clicking and holding in the column header and choosing the alignment mode from the Align submenu of the Property shortcut menu.

**Displaying the Entry Name.** You can display the entry name in the scrolling area of the table by choosing Show Entry Name from the Property menu. This option can also be set as a preference in the Project tab of the Preferences panel.

**Setting the precision of real values.** You can set the precision of real-valued properties in the Set Precision dialog box, which you open from the Property menu.

## 9.4.8 Navigating the Project Table

There are several means of navigating the Project Table rows. The UP ARROW and DOWN ARROW keys scroll the rows. You can use the HOME and END keys to go to the top and bottom of the table, and the PAGE UP and PAGE DOWN keys to move up and down the table a page at a time. The scroll wheel scrolls the table one row at a time, and in combination with the SHIFT key, scrolls one page at a time.

Special key bindings have been provided to traverse groups. To move to the top of the next or previous group, use the SHIFT key in combination with the UP ARROW and DOWN ARROW keys. To move to the top of the next or previous group, expand the group, and collapse all other groups, use the CTRL key in combination with the UP ARROW and DOWN ARROW keys.

These and other key bindings are summarized in [Table 9.6](#).

## 9.4.9 Finding and Replacing Text in the Project Table

If you want to locate text or replace text in the Project Table, whether it is a string or a numerical value, choose Find/Replace from the Table menu, press CTRL+F, or click the Find/Replace toolbar button.



The Find toolbar is displayed. By default it is located above the status bar at the bottom of the panel, but you can drag its handle to place it wherever you want.

Enter the text you want to find in the Find text text box, and click Next or Previous to search down or up. The Project Table scrolls to the found entry. The text is selected in the table cell and highlighted in green. All other occurrences are highlighted in yellow. The highlighting remains until you hide the toolbar. The number of matches is displayed on the status bar when the search is first performed.

To find the next occurrence of the text, click Next or Previous again. The Project Table scrolls to the next instance of the search string. The search wraps when it reaches either end of the Project Table.

You can choose to match the case of the search text exactly, by selecting Match case on the Options button menu, or to match the search text as a whole word, by choosing Match whole word only. For example matching “protein” as a whole word would not match “proteins”.





By default, the entry that is found is *not* selected, so that searching for text does not change the entry selection. If you want to select the found entries, select **Select entries with matches** on the **Options** button menu.

To replace text, enter the old text in the **Find text** box and the new text in the **Replace with text** box, then start the search. When you have located the text, click **Replace**. The text is replaced and the next occurrence of the search text is located. Clicking **Replace** instead of **Next** before you have found the search text finds the first occurrence, but does not replace it.

To replace all occurrences of a piece of text with new text, enter the old text in the **Find text** box and the new text in the **Replace with text** box, then click **Replace All**. The text is replaced, and a dialog box is displayed that reports the number of occurrences replaced.

You can restrict the search range to selected rows by selecting **Selected rows only** on the **Options** button menu. The selected rows are the entries that are selected in the **Project Table**, which you can change in the **Project Table** itself. If you want to limit the range of properties, select **Selected properties only** on the **Options** button menu, and choose the properties you want to search in the **Select Property** dialog box.

By default, the search includes entries in groups that are expanded (entries displayed), but not in groups that are collapsed (entries not displayed). You can search all groups by selecting **Search in collapsed groups** on the **Options** button menu.

## 9.5 Selecting Project Entries

Selection means choosing entry rows in the **Project Table**, which become the target for an action. The rows are highlighted when they are selected. Selection differs from “inclusion,” which is the display of the structures belonging to entries in the **Workspace**. Inclusion is described on [page 183](#). Selection is no different in principle from the selection of items in a list in any graphical interface. In addition to the usual mouse operations, summarized in [Table 9.1](#), **Maestro** provides capabilities for selecting entries based on their properties. Selection can include one or more entry groups.

Once entries are selected, they can be operated on using the mouse or the tools in the **Entry** menu. Selected entries can be renamed, duplicated, combined, split, deleted, exported, and included in the **Workspace**, or a movie of the structures associated with entries can be made with the **ePlayer**. Some operations on selected entries are mapped to shortcut keys, which are described in [Table 9.5](#) on [page 192](#).

Selection states are persistent across **Maestro** sessions: entries that are selected when a project is closed will still be selected the next time that project is opened. When new entries are imported or incorporated into the **Project Table**, they are automatically selected.

## 9.5.1 The Select Menu

The Select menu provides tools for selecting entries. The first three items, All, None, and Invert, select all entries, no entries (deselect all entries), and invert the selection (select the unselected entries, and deselect the selected entries). Only, Add, and Deselect open the Entry Selection dialog box, so that you can select entries by a combination of properties. By SMARTS allows you to select entries that match a SMARTS pattern; From Groups allows you to select the same selection criteria to multiple groups; Random allows you to randomly select a number or a percentage of entries. These last three items all open dialog boxes to make the selection.

The Filter submenu allows you to choose a named *filter* that is used to select entries, and to edit named filters. Filters are defined in terms of Entry Selection Language (ESL) expressions, and do not constitute a fixed set of entries. Whenever the filter is used, the ESL expression is applied to the current contents of the Project Table. For more information on ESL, see the *Maestro Command Reference Manual*.

## 9.5.2 Selecting Entries By Property

The Entry Selection dialog box (Figure 9.3) enables you to select entries in the Project Table based on a combination of criteria for property values. Once you have defined a set of criteria for selecting entries, you can store this set as a named filter, and use the filter directly from the Select menu. You can open the Entry Selection dialog box from the Select menu by choosing Only, Add, or Deselect. Only, Add, and Deselect. The Entry Selection dialog box is similar in design to the Atom Selection dialog box. It allows you to select entries using GUI tools rather than entering an ESL expression.

At the top of the entry selection dialog box is a title bar, which defines the action to be taken when you click OK. In the center are two tabs, Properties and Filters, that you use to define property-based criteria for entry selection or choose named filters to combine with the entry selection that is being created (the *current* entry selection). On the right are buttons for combining the criterion or named filter with the current entry selection. These tools become available when you have selected a property and a condition for that property, or a named filter. In the lower portion of the panel is an ESL text box that displays the current entry selection and a set of buttons for editing the current entry selection.

To define a property criterion, choose a property from the list in the Properties tab, then select a condition from the right side of the tab. The list can be restricted by choosing a subset, filtered, or sorted. The available conditions depend on the property type. For some conditions, you must enter a value or a range of values. The available conditions are:

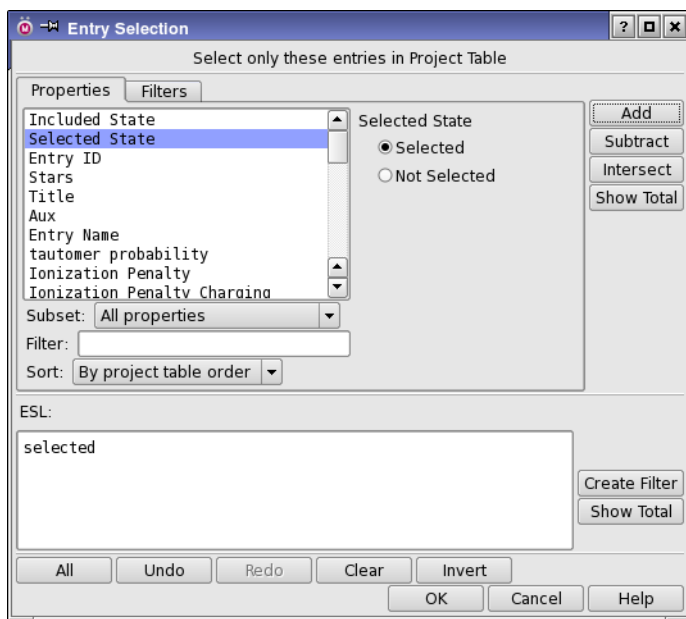
- The property is defined.
- For Boolean properties, the value is true or false.

- For numerical (real or integer) properties, the value lies in a given range, for example,  $\geq 5.0$  or  $1 - 7$ . You can use any of the six operators  $=$ ,  $\neq$ ,  $<$ ,  $>$ ,  $\leq$ , and  $\geq$  to define the range of property values.
- For string properties, the text matches a given string. “Match” means that the string given is contained in the property value. The string can include the wildcard characters  $*$ , which matches any number of characters,  $?$ , which matches any single character, and  $\#$ , which matches any single digit.

In addition, the inclusion state and the selection state of the entry can be used as criteria.

To combine this criterion with the current entry selection, click one of the buttons to the right of the panel.

- Add adds entries that meet the new criterion to the current entry selection, using a logical OR operation on the ESL expressions. This is the default action, which is performed if you press ENTER.
- Subtract excludes entries that meet the new criterion from the current entry selection, using a logical AND NOT operation on the ESL expressions. If this is the first operation, the default current entry selection is all.
- Intersect limits the selection of entries to those in the current entry selection that also meet the new criterion, using a logical AND operation on the ESL expressions.



**Figure 9.3.** The Entry Selection dialog box.

In addition to these three buttons, the Invert button at the bottom of the panel inverts the entire current entry selection, using a logical NOT operation. All entries that were selected are unselected, and all entries that were not selected are selected.

You can undo multiple operations with repeated clicks on the Undo button. The Redo button reverses undo operations, and can also be used multiple times. You can also type ESL expressions directly into the ESL text box. The hand-edited expressions are considered part of the last operation performed with the mouse and can be undone and redone as part of that operation, but cannot be undone or redone separately.

Once you have defined the criteria for selecting entries, the current entry selection can be stored as a named filter. To create a filter, click Create Filter. The New Filter dialog box opens, in which you can provide a name for the filter. The newly created filter appears in the Filters tab of the Entry Selection dialog box and on the Filter submenu of the Select menu.

### 9.5.3 Selecting Entries By Matching a SMARTS Pattern

You can select entries that match one or more SMARTS patterns, in the Select by SMARTS panel, which you open by choosing Select → By SMARTS. The search can be run on all entries or on the selected entries. If it is run on all entries, the matches can be added to the selection or they can replace the selection. These choices can be made with the Search option menu. SMARTS patterns can be combined with logical operators, which are processed in sequential order from the top, applying the logical operation at each step. You can highlight the atoms that match the SMARTS expression in the selected entries by selecting Highlight atoms.

**To select entries that match a single SMARTS pattern:**

1. Enter the SMARTS pattern in the text box at the top of the panel, or select atoms in the Workspace and click Get from Workspace Selection.
2. Choose a search scope and action from the Search option menu.
3. Click Select.

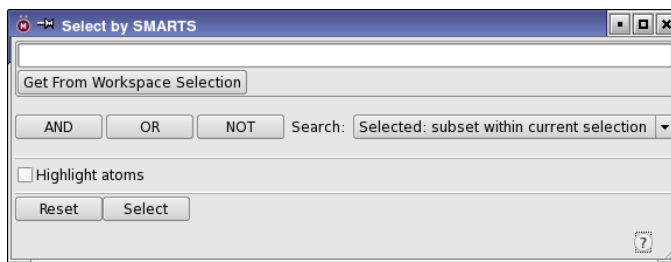


Figure 9.4. The Select by SMARTS panel.

**To construct a complex search expression with several SMARTS patterns:**

1. Enter the SMARTS pattern in the text box at the top of the panel, or select atoms in the Workspace and click Get from Workspace Selection.
2. Click AND, OR, or NOT.

Another section containing a SMARTS pattern text box and Get from Workspace Selection button is added above the logical operator buttons.

3. In this new section, enter the SMARTS pattern in the text box, or select atoms in the Workspace and click Get from Workspace Selection.
4. To add another SMARTS pattern, repeat from step 2.
5. When all SMARTS patterns are entered, click Select.

To clear all the SMARTS patterns, click Reset. If you get the SMARTS pattern from the Workspace selection, you can set preferences for some of the notational elements in the generated SMARTS pattern—see [Section 14.14 on page 375](#).

### 9.5.4 Selecting Entries Using the Plot Panel

The Plot panel provides a means of graphically selecting entries and including them in the Workspace. By plotting a property value against the entry name, for example, you can view the properties and select the entries on the plot that you are interested in. See [Section 11.1.5 on page 289](#) for more information.

### 9.5.5 Selecting Entries Using the 2D Viewer Panel

The 2D Viewer panel provides an alternative method for selecting entries on the basis of their 2D structures. The structures are presented in a grid, and you can synchronize the selection of structures in the grid with the Project Table selection. You can also change the inclusion state in this panel. See [Section 9.9 on page 220](#) for more information.

### 9.5.6 Selecting Entries Randomly

You can make a random selection from the entries in the Project Table by using the Random Selection dialog box, which you open by choosing Select → Random. The set of entries from which the random selection is made can be based on the selected entries or groups, or all entries or groups, and you can select a number of entries or a percentage of entries. For percentages, the number of entries selected is rounded to the nearest integer. If you choose to select from entry groups, the random selection is made from each group. Otherwise the random selection is made from the entry selection without regard to groups. The number of entries or groups from which selection is made is indicated next to the controls.

## 9.5.7 Selecting Entries in Groups

When you select an entry group, all the entries in the group are selected, and all other entries are deselected. You can use shift-click and control-click to select multiple groups, and the entries in these groups are selected. The group row is colored a light brown if all its entries are selected, and white if none of its entries are selected.

You can make selections of a specified number or percentage of entries in one or more groups by choosing **Select** → **From Groups**. In the **Select from Groups** dialog box, you can set the number or percentage of entries to select, starting from the first or the last entry in the group. The selection can be taken from the currently selected groups or from all groups. This feature is useful if you have sorted the entries in the group by a property and want to select entries with the highest or lowest values of the property. You can also make random selections—see [Section 9.5.6 on page 201](#).

The **Group** menu offers two selection items. If you select some but not all entries in one or more groups, you can invert the selection inside each group that has selected entries by choosing **Invert Selection** from the **Group** menu. The group rows for these groups are colored light orange. You can also deselect all entries that are inside groups without affecting the selection of single groups by choosing **Deselect All** from the **Group** menu.

## 9.5.8 Selection Examples

There are generally multiple ways to perform each selection operation: from an option on the **Select** menu, using the **Entry Selection** dialog box, using the mouse, and using ESL. A few examples of the use of the **Entry Selection** dialog box are provided here.

### **To select a range of entries with the same base name:**

1. Choose **Only** from the **Select** menu.
2. Select **Entry name** from the **Properties** list.
3. Select **Matches** in the conditions section and enter *entry\_name\** in the text box, where *entry\_name* is the base name of the entries you want to select.
4. Click **Add**, then click **OK**.

### **To add entries from the Workspace to the current selection:**

1. Choose **Add** from the **Select** menu.
2. Select **Included State** from the **Properties** list.
3. Select **Included** (or **fixed**) in the conditions section.
4. Click **Add**, then click **OK**.

## 9.6 Operating on Entries

The Entry menu provides tools to perform various operations on the selected table entries. These operations are discussed in the following sections. The Entry menu items are the same as the shortcut menu items, which are described in brief in [Table 9.3](#).

### 9.6.1 Including, Excluding, and Fixing Entries

In addition to using mouse operations, you can include and exclude entries in the Workspace by selecting the entries and choosing Include, Include Only, or Exclude from the Entry menu. The last two of these menu items are mapped to the shortcut keys CTRL+N and CTRL+X. You can also include and exclude entries by property value from a plot in the Plot XY panel. See [Section 11.1.5 on page 289](#) for more information on this feature.

If you want to keep some entries in the Workspace while including and excluding other entries, such as a receptor and a set of ligands, you can select the entries you want to keep in the Workspace and choose Fix from the Entry menu or the shortcut menu, or press CTRL+F. These entries remain in the Workspace until you explicitly exclude them, clear the Workspace, close the project, or choose Unfix from the Entry menu or the shortcut menu. Unfix removes the “lock” on the entries so that they are included in the Workspace but not fixed.

To fix a receptor in the Workspace (defined as an entry with more than a ligand-sized number of atoms), click the Fix button on the Style toolbar in the main window. Clicking again unfixes the entry (or entries).



For entries that are in an entry group, the Group shortcut menu offers some inclusion options. You can include all entries in the group by choosing Include All: the entries are added to the Workspace. Similarly, you can exclude all entries in the group by choosing Exclude All. If you want to include only the entries in the group, choose Include Only All. Finally, you can include the first entry in the group by choosing Include First.

There are several ways of stepping through entries in the Workspace, that is, including the next entry or the previous entry in the Project Table and excluding the current entry. If you have an entry selection, and one of these entries is included in the Workspace, you can use the LEFT ARROW and RIGHT ARROW keys to include the previous or the next selected entry in the Workspace and exclude the current entry. If you have more than one entry included in the Workspace, using the LEFT ARROW and RIGHT ARROW keys replaces each included entry in the Workspace with the next selected entry in the Project Table. Thus, you can step through multiple entries simultaneously to display them together in the Workspace. The other ways of stepping through entries are related, but have extra capabilities: the ePlayer ([Section 9.7 on](#)

page 216) and the pose viewing facility (Section 9.8 on page 219).

To exclude all entries from the Workspace, choose **Workspace** → **Clear** or click the **Clear** button on the **Workspace** toolbar:



This action also removes fixed entries from the **Workspace** and clears the scratch entry.

If you include multiple entries in the **Workspace** in a single operation, there is a chance that your computer does not have enough memory to store them all, particularly if they are proteins. A warning dialog box opens if you include more than a designated number of entries in the **Workspace**, and allows you to cancel the operation or to continue with the inclusion. You can adjust the number of entries at which the warning is displayed in this dialog box. If you continue, a progress dialog box is displayed if the inclusion takes more than a few seconds. You can stop the include operation at the last entry included by clicking **Stop** or pressing **ESC**. The entries already included remain in the **Workspace**.

### 9.6.2 Renaming Entries

When importing entries from files, incorporating entries from jobs, merging entries with identical names, duplicating entries, or disassociating entries, **Maestro** automatically assigns new entry names. You do not have to accept the automatically assigned names; you may rename the entries using one of the methods described below.

#### **To change the name of a single entry:**

1. Double-click the entry name if the entry is not selected, or single-click the name if the entry is selected.
2. Type in the new name.
3. Press **ENTER**.

#### **To rename multiple entries with the same name:**

1. Select the entries to be renamed.
2. Click the entry name for one of the entries.
3. Type in the new name.
4. Press **CTRL+ENTER**.



### 9.6.3 Locking Entries

If you do not want entries to be changed or deleted, you can lock them by selecting them and choosing **Entry → Lock**. A padlock icon is placed next to the row number. Locking entries means that the structure and the properties as stored in the project cannot be changed or deleted until you unlock them with **Entry → Unlock**. You can also use the **Entry** shortcut menu to lock and unlock entries.

- Jobs run from a locked entry with **Replace** as the incorporation mode will not replace structures or add properties, but can add surfaces. The job is marked as incorporated even though the structure and properties are not updated.
- You can edit the structure for a locked entry in the **Workspace**, but it will not be saved in the project. If you exclude the structure from the **Workspace**, any changes are lost.
- Attempting to delete a locked entry will not delete structures or properties, but will delete associated data.
- Locked entries can be sorted or moved around in the **Project Table**, because the position in the **Project Table** (row number) is not a property of the entry.

### 9.6.4 Duplicating Entries

To duplicate entries, select the entries and choose an item from the **Duplicate** submenu of the **Entry** menu. The possible choices are:

- **In Place**—Each duplicated entry is placed immediately below its source entry, and is included in the source's entry group if one exists. You can also use **CTRL+D** to duplicate entries in place.
- **Ungrouped**—Each duplicated entry is placed at the end of the ungrouped entries, in sequential order.
- **Into New Group**—The duplicated entries are placed into a new entry group. You can name the group in a dialog box that is displayed.
- **Into Existing Group**—The duplicated entries are placed into an existing entry group. You can select the group in a dialog box that is displayed.

To duplicate an entire entry group, right-click in the group row and choose **Duplicate**.

The new entries retain the same title and entry name as the originals. The duplicates are selected in the **Project Table** in place of the original entries, and any original entry that is included in the **Workspace** is replaced in the **Workspace** by its duplicate. If modifications have been made in the **Workspace** to any of the original entries, synchronization of the **Workspace** with these entries is performed according to the synchronization preference (see [Section 14.2.3](#)

on page 339). Any changes that were made to the Workspace that were not synchronized are transferred to the duplicated entries.

### 9.6.5 Merging Multiple Entries

Maestro allows you to merge two or more selected entries, while leaving the original entries unmodified. To merge entries, select the entries and choose Entry → Merge. When you merge entries, Maestro places the new entry after the last entry that was included in the merge operation (inside an entry group, if this entry is in a group). The entries are placed in the new entry in the order in which they appear in the Project Table. This order affects the atom and molecule numbers in the merged entry. You can control the order of addition by moving the entries in the Project Table before merging them.

Properties are also copied to the new entry. The properties of the entry with the most atoms (the “lead” entry) are copied first, then the properties of other entries are added, in Project Table order, to any blank cells. The title of the new entry is a concatenation of the titles of the source entries, lead entry first, then the others in Project Table order. If more than three entries are merged, the lead title is used with a suffix `_mergedN`, where *N* is the number of merged entries. The entry name is likewise merged. Auxiliary data is not copied.

An alternative way of creating a new entry from several existing entries is to include them in the Workspace, then create an entry from the Workspace. The order in which the entries appear in the new entry is the order in which they were included in the Workspace.

If you want to merge entries in the order of their entry IDs, enter the following command in the Commands text box in the main window:

```
entrycombine order=entryid
```

### 9.6.6 Copying and Pasting Entry Properties

You can copy properties from a selected entry to the clipboard, and paste them into a selection of other entries, either in the current project or another project.

To copy properties, use Entry → Copy Properties, and choose All to copy all properties, or Shown to copy the properties that are shown in the Project Table.

To paste properties, select the entries you want to paste the properties into, and choose Entry → Paste Properties. The properties from the clipboard overwrite any existing properties of the same (internal) name. If a property does not exist (or is of a different type) a new property is created and values added for the selected entries. If a property value is empty in the source entry, it overwrites values in the target entries with an empty value.

## 9.6.7 Splitting Entries

Entries that contain multiple molecules or chains can be split into entries that contain individual molecules. For example, you can split a protein-ligand complex into separate entries for the protein, the ligand, and the waters. To split an entry, select it and choose Entry → Split, then By Molecule, By Chain, or Into Ligands, Water, Other. When an entry is split, the original entry is kept, and a new entry is created for each molecule, chain, or other entity in the original entry.

If the entry has zero-order bonds, splitting the entry does not break these bonds by default. You can set a preference to determine whether zero-order bonds are considered when deciding which atoms belong to the same molecule—see [Section 14.11.1 on page 365](#) for details. You can also delete the zero-order bonds before splitting, from the Delete button menu on the Edit toolbar.



Some applications, such as the Protein Preparation Wizard, create zero-order bonds that are broken by default, overriding this preference. If you have a metalloprotein, for example, the Protein Preparation Wizard converts it into an ionic form, replacing any covalent bonds to the metal with zero-order bonds. Splitting such a complex by molecule separates the metal from the protein.

The new entries inherit the title of the original entry, with a suffix that indicates what kind of structural unit is in the new entry. The entry names are also modified from the original by adding a suffix. When you split by molecule, water molecules are collected in a single entry, with the suffix `_waters`. The molecule entry names have the suffix `_moln`, where *n* indexes the new entries; the title suffix is `_moleculen`. When you split by chain, the new titles have the suffix `_chainX`, the entry names have the suffix `_chain-name`, and a Chain Name property is created to store the chain name. When you split into ligands, water, and other, the entry name suffixes are `_ligandn`, `_waters`, and `_others` (entry name) or `_protein` (entry title).

If you want to copy the properties of the original entry to the new entries, choose Entry → Split, and then select Copy Properties.

## 9.6.8 Grouping Entries

You can create groups of entries, and perform operations with the groups as a whole or restrict operations to the members of a group. Entry groups are listed at the end of the Project Table, and are identified by a group title and index. The number of entries in the group is given in square brackets at the right of the Title column, and the entry group index is given in the title column before the group title. The groups are stored as part of the project. Entry groups can be created automatically when you import multiple structures, and use the file name (without the

suffix) for the group title. They can also be created automatically when multiple structures are incorporated as part of job output, and use the job name as the group title.

You can create an entry group by selecting entries, then choosing **Group → New** from the **Entry** menu or the **Entry** shortcut menu. A dialog box is displayed, in which you can enter the title of the group. When you create the group, it is added at the end of the table, and the entries you selected are moved inside the group.

To reorder groups, select them in the table and drag them to the desired location.

Another means of grouping entries is to group them by the value of a particular property. If you want to create a single group for a value or a range of values of a property, you can use the **Entry Selection** dialog box to select the entries, then choose **Create Group** from the **Entry** menu to create the group. If you want to create multiple groups, choose **Entry → Group → By Entry Property**, which opens the **Group By Entry Property** panel. You can choose the property from the **Property** list, which you can filter and sort, and group all entries or the selected entries.

- For string properties, a group is created for each unique string.
- For Boolean properties, two groups are created, for **TRUE** and **FALSE** values of the property.
- For real and integer properties, the range of property values is divided into “bins” of a specified size and entries are assigned to the bins on the basis of the property value. If you choose a real or integer property, these controls for the range and the bin size are shown:
  - **Step Size**—Size of the bins used to divide the entries into groups. The bins include the lower end of the range of values but exclude the upper end: thus a bin of size 2.0 for a real property starting at 2.0 would cover the range  $2.0 \leq \text{value} < 4.0$ .
  - **Align on value**—Reference point for the lower end of each bin. The lower end of each bin is set to this value plus (or minus) a multiple of the step size. For example, if the reference point is 5 and the step size is 3, there will be bins covering the ranges 2–4, 5–8, 9–11, and so on. If this option is deselected, the reference point is the minimum of all values of the property in the entries that are to be grouped. This option is on by default, with the value zero.
  - **Minimum**—Lower limit for property values to be considered. Entries whose value of the selected property is less than this limit will not be grouped.
  - **Maximum**—Upper limit for property values to be considered. Entries whose value of the selected property is greater than this limit will not be grouped.

To create the groups, click **Group**. You can enter an optional base name for the group, which is used to construct the group title by adding the property name and information on the property values in the group to the base name.

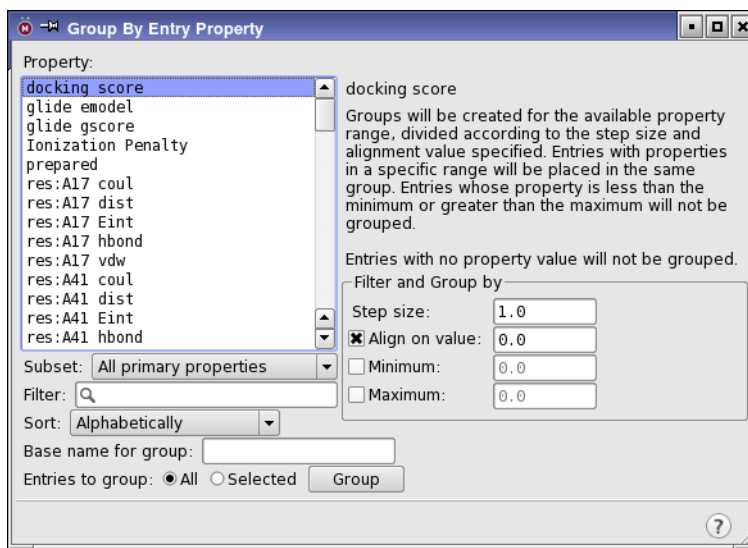


Figure 9.5. The Group By Entry Property panel.

If you want to change the group title, you can double-click on it and edit the text in the table cell, or you can right-click on the title cell and choose Edit Title.

### 9.6.9 Showing And Hiding Entries in Groups

The entries inside entry groups can be shown in the table (the group is *expanded*), or hidden (the group is *collapsed*). You can expand or collapse a single group by clicking in the In column. For multiple groups, you can show or hide the selected entry groups or all entry groups from the Expand and Collapse submenus of the Group menu, or from the Group shortcut menu, by choosing Selected or All. You can also expand the selected groups and collapse all others by choosing Only Selected from the Expand submenu. The visibility of entries in groups has no effect on their selection or inclusion state.

### 9.6.10 Deleting Entries

You can delete entries from the Project Table by selecting the entries, then choosing Delete from the Entry menu or pressing DELETE. You are prompted to confirm the deletion, but you can choose not to be prompted in the confirmation dialog box. Entry deletion can be undone by selecting Undo entrydelete from the Edit menu in the Maestro main window.

You can delete entry groups in the same way, by selecting the groups then choosing Delete from the Entry menu or pressing DELETE. The entries are deleted from the groups immediately, and then you are prompted for removal of the empty entry groups. If you have multiple

empty groups, you can delete them all by choosing Delete All Empty Groups from the Group menu.

### 9.6.11 Moving Entries

Entries in the Project Table can be moved to another location in the table. Multiple entries can be moved simultaneously, and entries need not be contiguous. To move entries, select them and then drag them to the desired new location. The entries are placed after the first unselected entry that precedes this location. For example, if you select entries 2, 4, and 6, and release the mouse button on entry 3, these three entries are placed after entry 1, because entry 1 is the first unselected entry that precedes entry 3. To move entries to the top of the table, drag them above the top of the table; to move entries to the end of the table, drag them below the end of the table. Dragging entries into an expanded entry group works in the same way as in the ungrouped section of the table. Dragging entries to the heading row for the entry group places them at the end of the group.

You can also move the rows that you have selected by choosing Move Rows from the Entry menu. In the Move selected entries to row dialog box, you can specify the starting row number for the first moved entry, or choose to move the rows to the beginning or the end of the table.

Entries that are inside a group can be moved out of the group or moved to another group. To move entries out of a group, select the entries, then choose Ungroup from the Entry menu to place them at the end of the ungrouped entries, or drag them to the desired location. To move entries to another group, select the entries, then drag them to the desired location in the new group, or choose Move to Group from the Entry menu. The Move To Group dialog box is displayed, in which you can select an existing group, select <no group> to ungroup the entries, or select <new group> and create a new group. If you move all the entries out of a group, a dialog box is displayed in which you can choose to delete or keep the empty group.

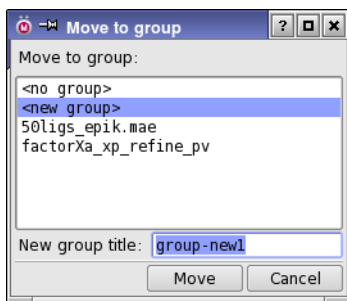


Figure 9.6. The Move To Group dialog box.

### 9.6.12 Sorting Entries and Entry Groups

You can sort project entries by property. For example, if you sort project entries in descending order based on their inclusion state, entries included in the Workspace are placed at the top of the list, and excluded entries are placed at the end. Sorting these entries in ascending order places included entries at the end of the list.

Sorting entries respects the grouping of entries: the ungrouped entries are sorted, and the entries within each group are sorted, but there is no change in the order of the groups or in the group membership.

The order in which string values are sorted can be changed with a preference. By default, sequences of digits are treated as a single number, so that, for example, `ligand10` follows `ligand9` rather than `ligand1`. If you want a standard dictionary sort, you can set a preference under Project Table – Properties in the Preferences panel—see [Section 14.3.1 on page 341](#).

To sort all entries by a single property, right-click and hold in the property header and choose Sort from the shortcut menu. If the sort order is not what you wanted, choose Sort again from the shortcut menu, and the entries are sorted in the opposite order.

To sort selected entries, to sort entries by more than one property, or to sort entry groups, you can use the Sort Project Table panel. In this panel you can choose as many sort keys as you want, and specify the sort direction. The panel also offers grouping before sorting, sorting of groups, and entry selection after sorting. These features are hidden by default.

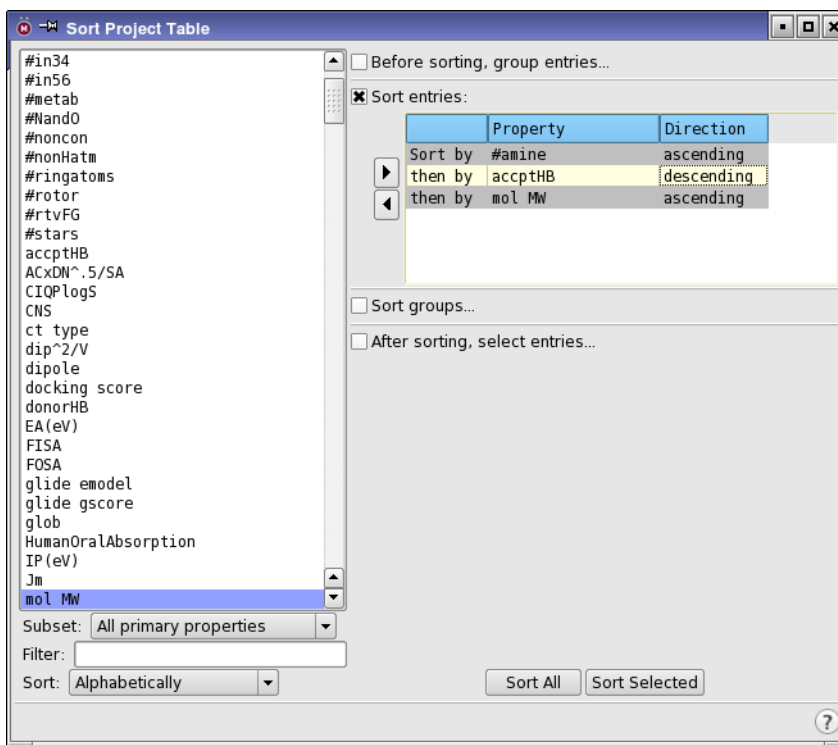
To open the Sort Project Table panel, choose Table → Sort or click the Sort toolbar button.



#### To sort entries:

1. Select a property from the list on the left, and click the right-facing arrow button in the center of the panel.  
The property is added to the Sort entries table.
2. Click in the Direction column for the property to change the direction of the sort.
3. To add another property, repeat [Step 1](#) and [Step 2](#).
4. To move a property up or down, select it and drag it to its new location.
5. Click Sort Selected or Sort All.

If you want to change the order of the entry groups, you can sort them by title or by the properties of their first entry.



**Figure 9.7.** The Sort Project Table panel, showing entry sorting tools only.

#### To sort entry groups by title:

1. Select Sort groups.

The controls for sorting groups are displayed below the option and the text of the option changes to Sort groups by.

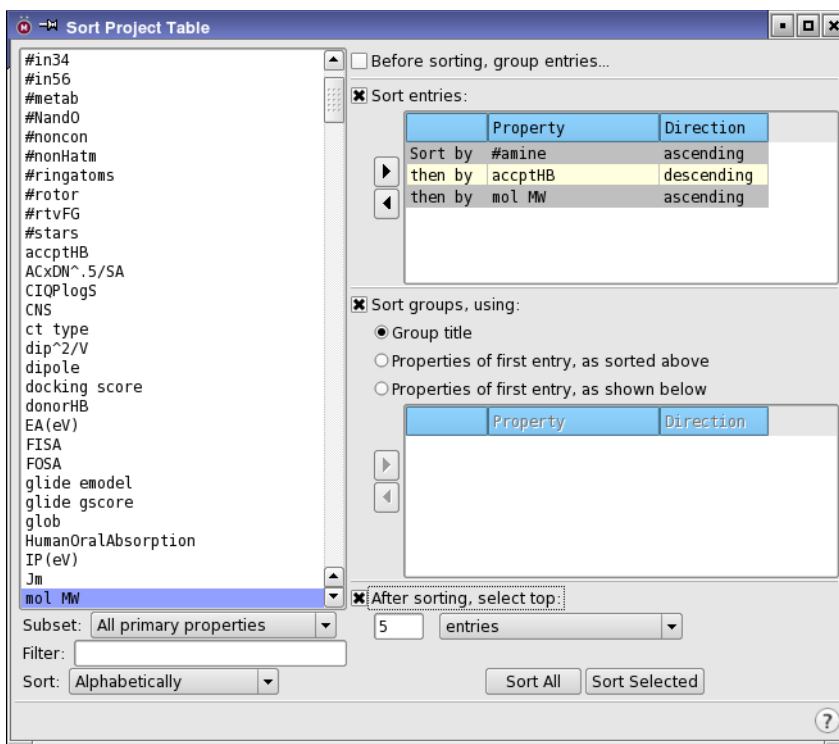
2. Select Group title.
3. Click Sort Selected or Sort All.

#### To sort entry groups by the properties of the first entry:

1. Select Sort groups.

The controls for sorting groups are displayed below the option and the text of the option changes to Sort groups by.





**Figure 9.8.** The Sort Project Table panel, showing all tools.

2. Select an option for the sort keys:
  - Properties of first entry, as sorted above—sort by the properties of the first entry using the same sort keys as for sorting the entries.
  - Properties of first entry, as shown below—sort by the properties of the first entry using the sort keys specified in the table below.
3. Select the properties for sorting and add them to the relevant table, setting the sort order and the sort direction, as necessary.
4. Click Sort All or Sort Selected.

You can group entries before sorting by selecting Before sorting, group entries, then clicking Options to set up the definition of the groups in the Group by Entry Property dialog box.

**To set up entry selection after sorting:**

1. Select After sorting, select entries.

The selection controls for entries are displayed.

2. Enter the number or percentage of entries to select in the text box.

The percentage is the percentage of the entries that were sorted.

3. Choose whether to select a number or percentage of entries, and whether to select them in each group or in the entire sorted set of entries, by choosing from the option menu.

**9.6.13 Ranking and Sorting Entries by Rank**

There are occasions when you may want to sort entries by a rank that is calculated as the optimum value of several properties, rather than sort them by properties independently. You can calculate a rank by the Pareto method for two to four properties, and then sort entries by this rank, in the Multivariate Ranking panel.

To open this panel, choose Table → Multivariate Ranking.

**To rank a set of entries by the optimal values of 2 to 4 properties:**

1. Click Choose and choose the properties.

The table is populated with the property names and the default action, which is Maximize. You can delete a property by right-clicking and choosing Delete.

2. If the best value of a property is the minimum, click in the Action column for that property to change it from Maximum to Minimum.

3. Enter a property name for the rank in the Save as property text box.

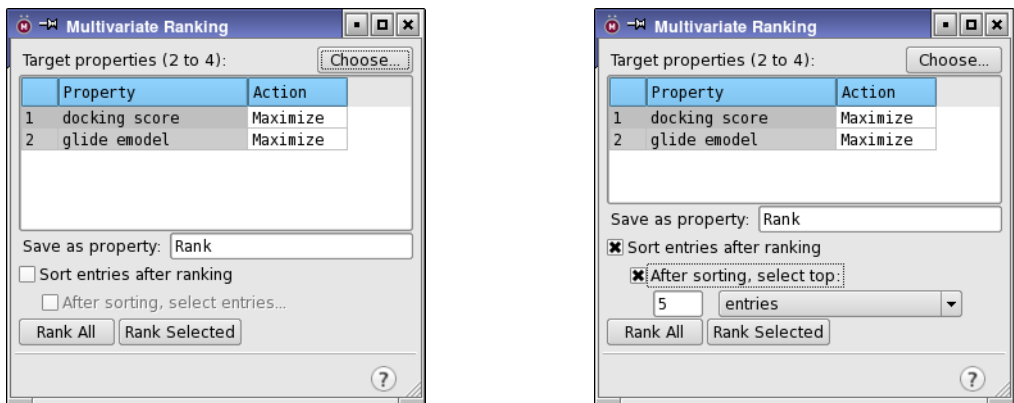


Figure 9.9. The Multivariate Ranking panel.

4. If you want to sort the entries after ranking them, select Sort entries after ranking. Entries within groups are sorted independently.
5. If you want to select the top-ranking entries after sorting, select After sorting, select entries. More tools are displayed, which allow you to choose an option for selecting from all entries or from each group, as a percentage or a number of entries, and enter the percentage or number in the text box.
6. Click Rank All to calculate the rank for all entries, or Rank Selected to calculate the rank for the selected entries. The sorting and entry selection is done, if the options were selected.

The rank value can be positive or negative. A large positive rank for an entry gives the number of entries that have a lower rank. A negative rank for an entry means that for this entry there are more entries with a higher rank than a lower rank. If the properties used in the ranking do not exist for an entry that is ranked, no value is calculated for the rank property, and it is left empty.

### 9.6.14 Recording a Movie from Selected Entries

Maestro provides a facility for creating an MPEG movie (MPEG-1) from the selected entries in the Project Table. To create the movie, select the entries, then choose Table → Record Movie. The Record Movie file selector opens, in which you can name the movie. By default the movie is recorded at 720×480 resolution with medium quality and a frame duration of 0.04 sec. If you want to select another resolution, change the quality, change the frame duration or total duration, or add interpolated frames to smooth the movie, click Options, and make settings in the Movie - Options dialog box. Adding interpolated frames increases the length of the movie: the frame duration remains the same.

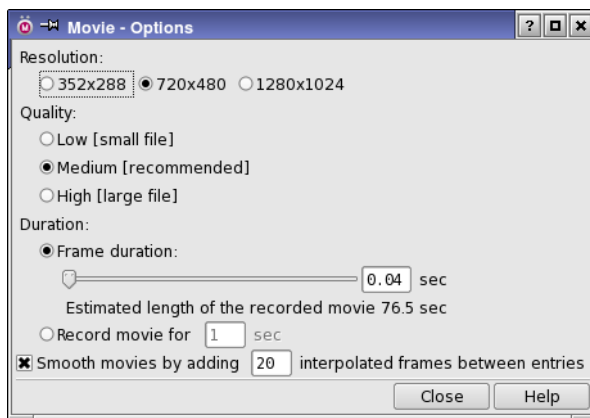


Figure 9.10. The Movie Options dialog box.

## 9.7 The ePlayer

The ePlayer allows you to view in succession the structures associated with selected entries. By carefully selecting entries to be included in the Workspace, and then selecting an entry to be used as a reference, you can use the ePlayer to visualize structure relationships such as ligand-receptor docking. You can also run a script on each entry as it is displayed. To use the ePlayer, you must have a project open with at least one entry selected. The ePlayer can be operated from the toolbar or from the ePlayer menu. The toolbar is hidden by default, but you can display it from the ePlayer menu (Show Toolbar). The toolbar buttons are described below.



**Go to start**  
Display the first selected structure.



**Previous**  
Display the previous structure in the list of selected structures. You can also use the LEFT ARROW key to display the next structure, either in the Project Table or in the Workspace.



**Play backward**  
Display the selected structures in sequence, moving toward the first.



**Stop**  
Stop the ePlayer. You can also press ESC to stop play.



**Play forward**  
Display the selected structures in sequence, moving toward the last.



**Next**  
Display the next structure in the list of selected structures. You can also use the RIGHT ARROW key to display the next structure, either in the Project Table or in the Workspace.



**Go to end**  
Display the last selected structure.



**Loop**  
Choose an option for repeating the display of the structures. **Single direction** displays structures in a single direction, then repeats. **Oscillate** reverses direction each time the beginning or end of the list is reached.

The ePlayer menu has two additional items that are not represented on the toolbar:

- **Next Group**—Include only the first selected entry in the next entry group.
- **Previous Group**—Include only the first selected entry in the previous entry group.

### 9.7.1 ePlayer Modes

The ePlayer has two modes, Continuous mode and Step mode. In Step mode, you manually advance the ePlayer to show each new entry structure. You can use the Next and Previous buttons on the toolbar, the Next and Previous items on the ePlayer menu, or the RIGHT ARROW and LEFT ARROW keys.



To go to the beginning or the end of the entry list, use the Go to Start or Go to End toolbar buttons or ePlayer menu items.



In Continuous mode the ePlayer automatically displays all selected entry structures in sequence. You can play through the structures once, or you can loop over the series by repeating the sequence of structures in the same direction, or by reversing the direction. You can stop play by pressing ESC. These options can be selected from the Loop submenu of the ePlayer menu or the Loop button menu on the toolbar.



If you choose None, the ePlayer displays the selected structures once in the direction you choose and stops.

If you choose Single Direction, the ePlayer displays all selected structures in sequence, then loops back to the first structure and redisplay the entire series until you click another ePlayer directional button.

If you select Oscillate, the ePlayer displays all of the selected structures in the forward direction, then in the reverse direction, and repeats this sequence until you click another ePlayer directional button.

### 9.7.2 ePlayer Options

The ePlayer Options panel provides access to controls for the ePlayer and extra actions that can be performed during play. To open the ePlayer Options panel, choose Options from the ePlayer menu. The panel has three sections: general options, options for superimposing structures, and options for running a script.

## General

You can adjust the speed at which the ePlayer moves through the specified structures by entering a value in seconds in the Speed text box. This is the time that each structure is displayed in the Workspace. The default is zero seconds per entry, which means that the speed of play is limited only by the speed of rendering of the structures.

In Continuous play mode, the structures are only temporarily displayed in the Workspace. By default, any changes in the structure are also temporary. However, you can save changes during play by selecting Save workspace at each step.

## Superimpose Entry

One instance in which you may find the ePlayer very helpful is in superimposing entries onto each other or onto a reference structure. For instance, when viewing ligands, you might want to view them superimposed on a receptor. You can do this by fixing the receptor in the Workspace but selecting only the ligands.

If you choose On Previous Entry, each entry is superimposed on the previous entry in the series. If you choose On Reference Entry, you must specify a reference entry, either by typing its name in the Reference text box, or clicking the Choose button and choosing an entry from the list. The reference entry can be any entry, but to view it during play, you must fix it in the Workspace.

If you choose to superimpose structures in Step mode, the project synchronization mode that you have selected in the Preferences panel is applied. If you have chosen Automatically for the synchronization mode, superimposing structures changes the coordinates of the structures involved. If you do not want to save the coordinates that result from using the ePlayer, choose Only When Specifically Requested for the synchronization mode.

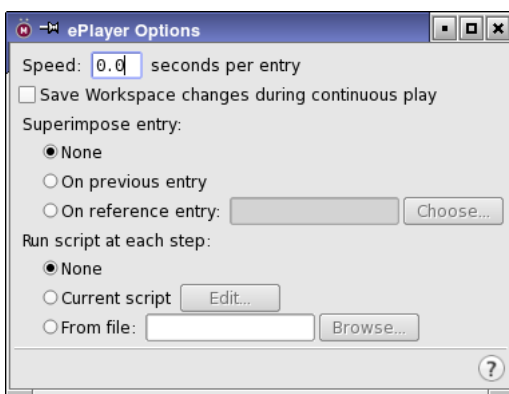


Figure 9.11. The ePlayer Options panel.

In Continuous mode, coordinate changes that result from superposition are saved to the project only if you have selected Save workspace at each step in the General section.

#### Run script at each step

In addition to superimposing structures, you can execute a command script when each structure is displayed. If you choose Current Script, the script that is currently loaded in the Command Script Editor panel is executed for each structure. You can open this panel and edit the script by clicking Edit. If you choose From File, you can choose the file that contains the command script you want to execute. This script is not loaded into the Command Script Editor panel, but is stored temporarily.

**Note:** You should not include in your script any command that operates on all selected entries, or that changes the inclusion state of the entries.

## 9.8 Viewing Poses

The Project Table panel provides a facility for viewing ligands that are aligned to a receptor active site, along with hydrogen bonds and contacts between the ligands and the receptor. When you set up pose viewing, the receptor and the ligands must be part of the same entry group, and the receptor must be the first entry in the selection (which need not include the whole group). You can subsequently add ligands in another group, for example, as the setup is done as a one-time action.

To start using the facility, chose View Poses from the Entry menu or the entry group shortcut menu and then click Set Up in the Pose Viewer panel. The receptor is fixed in the Workspace, the view is zoomed to the ligand, and a boolean property named Mark is added to the Project Table. You can step through the entries by simply including them in the Workspace, by using the ePlayer controls, or by using the LEFT ARROW and RIGHT ARROW keys. You can mark entries (or clear the mark) by pressing the X key. The Mark property is then set to TRUE, and displayed as a check mark in the Mark column. You can then select entries using this property.

The Pose Viewer panel also allows you to turn on or off the display of nonbonded interactions such as H-bonds and contacts, to generate counts of nonbonded interactions as Maestro properties, to set up nonbonded interactions using the Non-Bonded Interactions panel, and to display and define per-residue interactions. The display of nonbonded interactions selected from this panel is linked to the selection in the H-Bonds and Contacts panel, so that the selections in both places are the same. For more information on nonbonded interactions, see [Section 10.2.2 on page 249](#) and [Section 14.8 on page 357](#). For more information on viewing poses and per-residue interactions, see [Section 6.1 of the \*Glide User Manual\*](#).

## 9.9 Viewing 2D Structures

Maestro displays 3D representations of structures in the Workspace, but there are occasions when it is more useful to see a 2D representation of the structures. The project facility provides two ways in which you can view the 2D representation of structures, which are described in the sections below.

### 9.9.1 Displaying 2D Structures in the Project Table

You can display the 2D structure in a column of the Project Table, which allows you to associate the structure with its properties in a more direct manner than including the structure in the Workspace. To do so, click the 2D Structure toolbar button, or choose Property → Show → Show 2D Structures.

#### 2D

The structures are displayed as the third column in the Project Table (or the fourth, if the Stars column is shown), labeled 2D Structure. The structures are actually images that are generated when they are displayed. You can change the size of the displayed structures by dragging the row margin in the Rows column to change the row height. You can also set preferences for the images under 2D structure in the Preferences panel—see [Section 14.10 on page 364](#). Structures with more than a specified number of atoms (default 200) are not displayed. For protein-ligand complexes, the ligand is displayed, with an icon in the top right to indicate that a protein is present but not represented in 2D. The ligand is detected with the settings in the Ligand Detection Settings dialog box—see [Section 7.6.3 on page 159](#) for details.

If you do not want to display 2D structures as a column, but still want to be able to see them when needed, you can set a preference to display the 2D structure in a tool tip when the pointer pauses in the Row column—see [Section 14.3.1 on page 341](#).

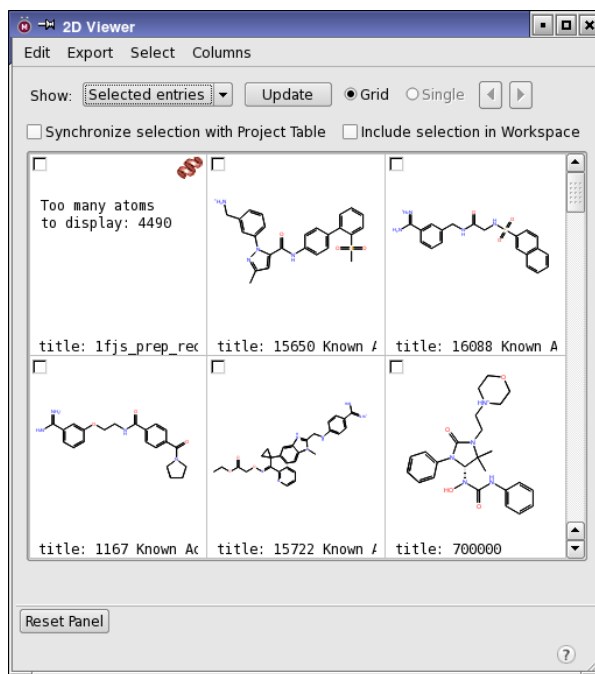
### 9.9.2 The 2D Viewer Panel

The second way of displaying 2D structures is to use the 2D Viewer panel. The basic function of the 2D Viewer panel is to display 2D representations of the structures in the Project Table and provide capabilities for selecting and including entries.

To open this panel, click the 2D Viewer button on the toolbar or choose Table → 2D Viewer (or click the 2D Viewer button on the Project toolbar or choose Project → 2D Viewer in the main window).







**Figure 9.12. The 2D Viewer panel.**

Like the 2D structures displayed in the Project Table, the 2D structures are images that are created when you open the panel, or when you click Update to update the panel contents from the Project Table. There may be a short delay while the images are generated. As for the Project Table display, images are not created for proteins or other large structures, but for protein-ligand complexes, the ligand is displayed, with an icon in the top right to indicate that a protein is present but not represented in 2D.

Each cell in the display area corresponds to an entry in the Project Table. The cells are arranged in a rectangular grid. The structures for the entries are added to the grid row by row: moving across a row and onto the next row is the same as moving down the Project Table. You can select the number of columns displayed from the Columns menu, and you can choose which entries are displayed from the Show option menu.

You can display selected properties at the bottom of each cell. By default, the title is displayed. To select the properties that are displayed, choose Edit → Select Properties. The 2D Viewer - Select Properties dialog box opens, in which you can select the properties that are displayed, and choose whether to display the property names. The dialog box provides standard tools for sorting the list of available properties and filtering it by product family or by text content.

In this dialog box, you can also choose an atom-level property to use to label atoms instead of the atomic symbol. All atoms, including carbon and hydrogen (if displayed) are labeled. After choosing a property from the Atom-level annotation property option menu, you must click Update in the 2D Viewer panel to see the chosen property on the atoms.

You can select cells with the usual shift-click and control-click actions, and you can drag to select cells. You can select all entries, clear the selection, and invert the selection from the Select menu. With a single cell selected, you can step through the structures with the arrow buttons, the arrow keys, with the N (next) and P (previous) keys, or from the Select menu.

The selection is independent of the selection in the Project Table by default, but you can make the panel selection and the Project Table selection the same by selecting Synchronize selection with Project Table. Selecting entries in either panel then changes the selection in the other.

If you have a single structure selected, you can display a larger image by selecting Single. To return to the grid display, select Grid. You can also switch between single structure and grid display by pressing ENTER.

The inclusion state is always the same as in the Project Table, and is indicated by the square in the top left of each cell. You can automatically include in the Workspace the structures that you select in the panel by selecting Include selection in Workspace. With this option, whenever you select a table cell, the structure is included in the Workspace.

The images that are used to display the 2D structures can be adjusted by setting preferences in the 2D structure group of the Preferences panel, which you can open by choosing Edit → 2D Display Settings. See [Section 14.10 on page 364](#) for details.

The images can also be exported in a variety of formats, from the Export menu. Each item on this menu opens a file selector in which you can navigate to a location and name the file.

- **Export to PDF**—Export the selected structures as images in a PDF file, in an array with the same number of columns as in the panel. The properties are included in the images with the structure. The images are exported as scalable vector graphics.
- **Export to PNG**—Export the selected structures to separate PNG files, named *base-MNN.png*, where *base* is the name that you specify in the file selector, and *MNN* is a serial number starting from 001. Only the 2D structure is included in the image.
- **Export to HTML**—Export the selected structures as PNG images included in a table in an HTML page, with the same number of columns as in the panel. The images are exported into a directory in the same location. If the file is named *myimages.html*, the image directory is named *myimages\_img* and the image files are named *myimagesN.png*, where *N* is an index starting from 1. The links to the images are relative, so the file and image directory can be moved to another location easily. The structure title is included as

alt text for the image. The properties displayed with the structure are included below the image in the HTML file.

- **Export to EPS**—Export the selected structures to separate encapsulated PostScript files, named *base-NNN.png*, where *base* is the name that you specify in the file selector, and *NNN* is a serial number starting from 001. Only the 2D structure is included in the image.

You can also copy the image of the selected cell (provided only one is selected) to the clipboard, with Edit → Copy or CTRL+C (⌘C)

In addition, the 2D structures can be exported to a 2D SD file, by choosing Export → Export to 2D SD. The 3D structures can be exported to an SD file with a SMILES string for the structure added as a property, by choosing Export → Export to 3D SD with SMILES.

There are some settings for exporting images and structures, which you can set in the 2D Viewer - Settings dialog box by choosing Edit → Settings.

- **Scale images on export**—Scale images to a uniform image size of 400×200 pixels when they are exported. Images are always scaled when exported to a PDB file. Deselect this option to produce images for which equivalent bonds have the same length.
- **When exporting, use transparent background**—Use a transparent background when exporting an image. The default is to use a white (opaque) background.
- **Include hydrogens when exporting to 2D SD format**—Include hydrogens in the 2D structure when exporting structures to a 2D SD file. The default is not to include hydrogens.

## 9.10 The Entry List Panel

The Project Table panel contains all the functionality in Maestro for access to projects and project data. For performing basic tasks, it is not always convenient to switch between the Workspace and the Project Table. A smaller, dockable panel that provides a basic view of the project is also available: the Entry List panel. This panel contains a reduced view of the Project Table, but retains many of the common capabilities, and is synchronized with the Project Table.

By default, the Row, In, and Title columns are shown. These columns are shown so you can include and exclude entries quickly without having to move your focus away from the Workspace. If you want to add a property column, right click on the table heading row and choose Show Property. A standard property selector opens, in which you can choose the property you want to show. To remove a property column, right-click on its heading and choose Hide.

Display of 2D structures is independent of the Project Table display, and can be done from the shortcut menu in the heading row.

Access to some of the Project Table functions is available through the shortcut menus, which duplicate those in the Project Table panel, except for a few items. See [Table 9.2](#), [Table 9.3](#) and [Table 9.4](#) for a description of these menus. You can use the keyboard to perform functions, such as including the next or the previous entry with the right and left arrow keys.

A feature that is not available in the Project Table panel is the ability to filter the list of entries shown in the Entry List panel. To filter the list by matching text, enter the text in the text box at the top of the panel. As you type, the list is filtered to include only the entries that have a match to the text anywhere in the title. Clicking the X button to the right clears the text and the filter.

You can also apply a filter based on the entry properties. Click and hold on the Filter button and choose from the menu that is displayed: Included to show only included entries, Selected to show only selected entries, or Filter to define a filter or choose a standard filter.

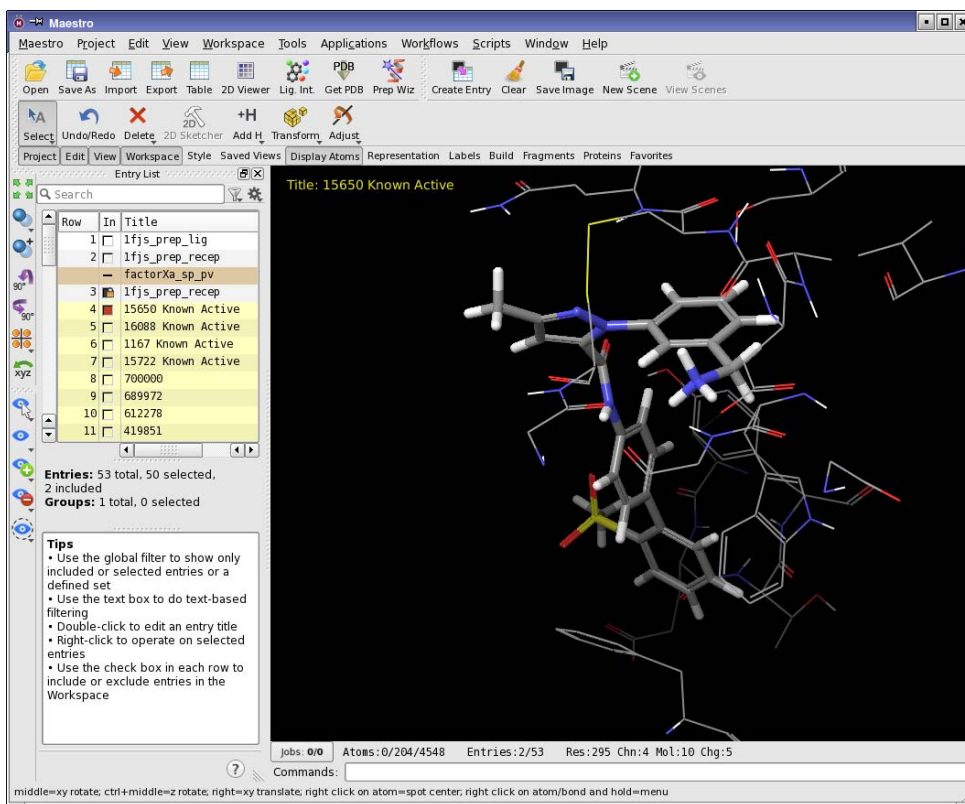


Figure 9.13. The Entry List panel docked into the Workspace.

When you choose Filter, the Entry Selection dialog box opens (see [Section 9.5.2 on page 198](#)), and you can set up and name a filter or choose an already named filter. The filter that you choose remains in effect (the Filter button is indented) until you click the button again. You can reapply the most recent filter that you selected by clicking the button: you do not need to select the item from the menu again. Both filters can be applied at the same time, and the filters are reapplied whenever the Project Table changes.

If you select multiple entries from a filtered list (with shift-click, for example), only the entries that are shown are selected. Any intervening entries that have been filtered out are not selected. The same applies to including entries in the Workspace from a filtered list: only the entries that are visible in the list are included in the Workspace.

Information on the entries in the project and the list is shown below the list: the number of entries and groups, the filter that is in effect and the number of entries shown after filtering on properties. A list of suggestions for the use of the panel is displayed at the bottom of the panel.

## 9.11 Entry Properties

Maestro supports incorporation and display of properties and calculated data for project entries. You can display, delete, sort, and filter entries based on property values. You can select a subset of properties to view, and you can add, delete, copy, and rename properties. Some properties of structures can be calculated by Maestro, such as the molecular weight, number of residues, and statistics of structural features. You can export properties to and import properties from a spreadsheet file. See [Section 3.3 on page 57](#) and [Section 3.4 on page 58](#) for information on exporting and importing properties.

Properties are displayed in columns in the Project Table. The property name is displayed in the column heading. If the property has units, these are displayed in the tool tip for the column heading, along with the property names (display name and internal name, see [Appendix E](#)).

Properties are classified into primary properties and secondary properties. These classifications are defined for each application that produces properties, but you can change the classifications. Only the primary properties are shown in the Project Table by default, but you can specify which properties are shown when adding entries by setting a preference—see [Section 14.3.1 on page 341](#).

Most of the operations you can perform on properties are available from the Property menu. Others, such as plotting, importing, and exporting, are available from the Table menu.

### 9.11.1 The Stars and Mark Properties

Maestro provides two special properties that you can use to rank and mark entries. One is the Stars property. This property allows you to give a ranking from zero to three stars to any entry. The property is displayed by default as the second column of the table. To set the number of stars, click on one of the stars. Click to the left of the stars to clear the star setting. You can also choose the number of stars from the Entry menu or the Entry shortcut menu, or use the 0, 1, 2, and 3 keys to set the number of stars for the selected entries. For a single (target) entry in the Workspace, you can use the \* key in the Workspace to cycle through the number of stars. The Stars property is an integer property with values from 0 to 3.

The other special property is the Mark property, which is a Boolean property. This property is set for the target entry when you press X, either in the Workspace or in the Project Table panel, or by choosing Entry → Mark → Target Entry. If the property does not exist, it is created. A check box is displayed in the Mark column for marked entries. The Entry → Mark submenu also allows you to mark the selected entries (Selected), the included entries (Included), and all entries (All); it also allows you to clear the mark for all entries (None) or to invert the marking of the selected entries, or all entries if there is no selection (Invert).

The target entry is the entry that is included in the Workspace that meets one of the following conditions:

- It is the only entry included in the Workspace
- It is the only entry included in the Workspace that is not fixed
- It is the only entry included in the Workspace that is selected

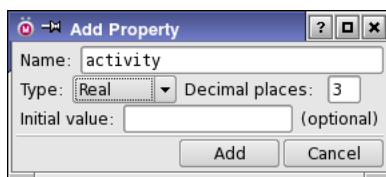
If you have single-entry feedback displayed in the Workspace, the target entry is the entry for which feedback is shown.

### 9.11.2 The Date Added and Date Modified Properties

When an entry is added to the project, two properties are added with it that record a time stamp: Date added and Date modified. The times are given in the local time in the form YYYY-MM-DD HH:MM:SS, and are stored as strings. The Date modified property is updated when changes to an entry are written to the project database. If you undo changes to the entry, the Date modified is also reverted to the previous value. When merging properties, the Date added property is set to the time of the merge.

### 9.11.3 Creating New Properties

Apart from incorporating results from a calculation and importing data from a spreadsheet, there are some ways in which you can create new properties. One is to add a property column and insert values into it manually. Another is to copy an existing property and modify the prop-



**Figure 9.14.** The Add Property panel.

erty values. A third is to calculate one of a selection of new properties. A fourth is to calculate a new property from existing properties.

### 9.11.3.1 Adding Properties with a Default Value

To add a property column to the Project Table, choose Add from the Property menu. In the Add Property panel, you can specify the name, the type, and the initial value of the new property (see Figure 9.14). When you add the property, all selected entries are assigned this property value. If you don't specify a value, the property is created but no values are assigned. For real-valued properties, you can set the precision to which the value is displayed. The default precision is set as a preference—see Section 14.3.1 on page 341 for more information.

### 9.11.3.2 Adding Properties by Copying

To create a new property by copying an existing property, choose Property → Copy to open the Copy Property panel. In this panel, select the property in the From list, select <Add New Property> in the To list, provide a property name in the New Property Name text box, then click All Entries or Selected Entries. A new property column is created, and the values are copied for all entries or for the selected entries. See Section 9.11.5 on page 232 for more information on copying properties.

### 9.11.3.3 Calculating Properties from Structural Data

Maestro provides a selection of properties that can be calculated for entries from the structure itself. These calculations are done from the Calculate Properties panel, which you open by selecting Property → Calculate. The available properties, given in the Property list at the top of the panel, are:

Chiral centers	AlogP
Molecular charge	Hydrogen bond acceptors
Molecular formula	Hydrogen bond donors
Molecular weight	Number of rotatable bonds
Number of atoms	Polar surface area
Number of heavy atoms	Molar refractivity

Number of molecules	Polarizability
Number of residues	Substructure
Spin multiplicity	Total surface area
Secondary structure content	Sequential index

For some properties, there are options or settings that must be made in order to calculate the property, such as a restriction on the number of atoms. These are presented in the Property Options dialog box, which opens when you click the button to calculate properties. To calculate properties, select them in the Property list, then click **All Entries** or **Selected Entries** under **Calculate *N* properties for**.

If you have previously calculated the properties for some entries and want to calculate them for other entries, you can choose to recalculate the existing values by selecting **Recalculate existing values**.

The **Chiral Centers** property choice calculates the number of chiral centers for ligand-sized molecules and adds the chirality properties used by LigPrep. These properties are calculated only for entries that contain a single ligand-sized molecule.

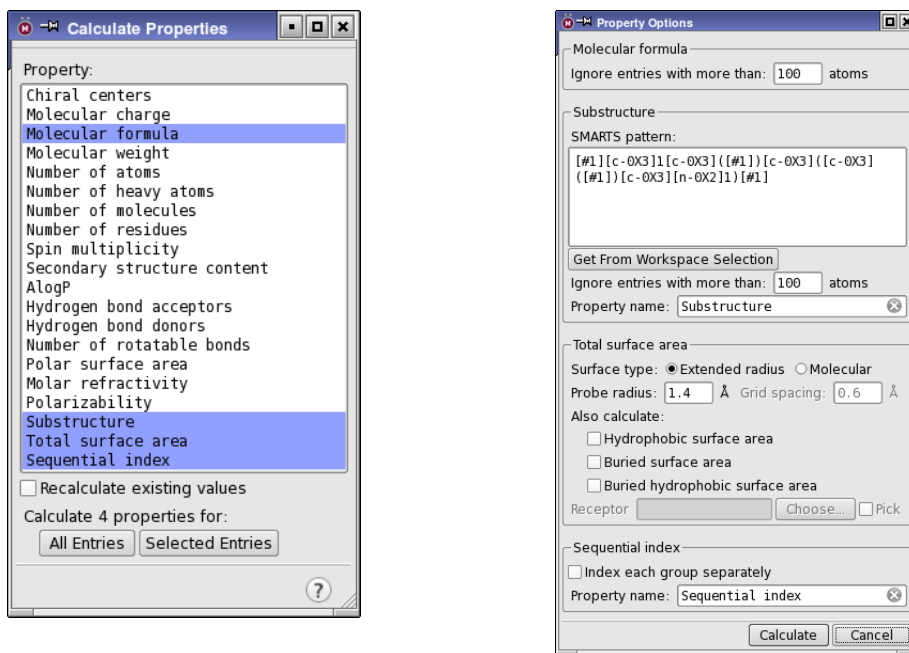
The **Secondary structure content** property is actually three properties: percentage of helices, percentage of beta strands, and percentage of random coils.

The **Substructure** property is the number of occurrences in each entry of the substructure that you provide (as a SMARTS pattern). You can specify the SMARTS pattern in the Property Options dialog box, either by typing or pasting it in, or by picking atoms in the Workspace and creating a pattern from the selection with the **Get from Workspace Selection** button. (You can set preferences for some of the notational elements in the generated SMARTS pattern—see [Section 14.14 on page 375](#).) You can also specify the property name.

The **Total surface area** property choice generates up to four properties, **Total Surface Area**, **Hydrophobic SA**, **Buried SA**, and **Buried Hydrophobic SA**. There are two options in the Property Options dialog box for the type of surface that is used: **Extended radius** or **Molecular**. These are the same as the surfaces available from the **Surfaces** submenu of the **Workspace** menu (see [Section 12.1.2 on page 297](#) and [Section 12.1.3 on page 298](#) for details). For each surface type, a probe radius must be given in the **Probe radius** text box. The default value of 1.4 Å is the value for water. For molecular surfaces you can also specify the grid spacing. Which surface area properties are generated depends on the options selected:

- **Hydrophobic surface area**—calculates the hydrophobic surface area of the molecule. Selecting this option produces the **Hydrophobic SA** property. Hydrophobic atoms are defined in the same way as for **Phase hydrophobic features**.





**Figure 9.15.** The Calculate Properties panel and Property Options dialog box.

- Buried surface area—calculates the buried surface area of the selected entries when a receptor is present. Selecting this option requires you to choose a receptor, and produces the Hydrophobic SA property.
- Buried hydrophobic surface area—calculates the buried surface area of a receptor when a ligand is present. Selecting this option requires you to choose a receptor, and produces the Buried Hydrophobic SA property.

For meaningful values of the buried surface areas, the entries that you calculate the property for should be docked to the receptor. The buried surface area is the area that is not solvent-accessible when the receptor is present.

When calculating buried surface areas, the Receptor controls enable you to choose a receptor. You can either pick a receptor in the Workspace, if Pick to define receptor is selected, or click Choose to choose an entry for the receptor.

For the Sequential index property, you can select an option to index the selected entries separately for each group. By default the index runs over all entries, regardless of grouping. You can also name the property.

### 9.11.3.4 Calculating Properties from Other Properties

In the Project Table Calculator Panel, you can construct formulas from arithmetic properties (real or integer), and use these formulas to construct new properties. The calculator provides the usual arithmetic operations and a range of mathematical functions and units conversions, as well as the ability to group expressions with parentheses to create complex formulas. The expression can be applied to multiple entries to create properties. To open the panel, choose Table → Calculator or click the Calculator toolbar button.

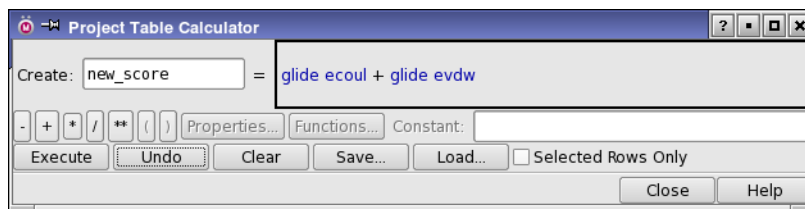


A formula can refer to any number of existing properties and functions, including mathematical functions. Formulae are assembled by using the operator buttons  $\sqrt{\quad}$ ,  $-$ ,  $+$ ,  $*$ ,  $/$ ,  $**$ , the parentheses buttons, the lists of properties and functions, and constants. Each time you click a button, a token is added to the formula, and the availability of the buttons is updated to reflect the valid choices for the next token.

- To add a property to the formula, click Properties. A dialog box opens that lists the available real or integer properties. Select the property, then click OK.
- To add a mathematical function to the formula, click Functions. A dialog box opens that lists the available functions. Select the function, then click OK.
- To add a constant to the formula, type the value in the Constant text box and press ENTER.
- To remove the last addition from the formula, click Undo. You can click this button multiple times to undo multiple additions to the formula.

The entire formula can be cleared by clicking Clear. There is no way to directly edit the formula.

When the formula is in a complete state the Execute button becomes available. This button evaluates the formula for all the rows in the current project, or if Selected Rows Only is selected then the formula is evaluated for only the selected rows in the Project Table.



**Figure 9.16.** The Project Table Calculator panel.

**Example: Calculating GlideScore divided by molecular weight.**

1. Calculate the molecular weight property:
  - a. Choose Property → Calculate in the Project Table panel.
  - b. Select Molecular weight from the Property list.
  - c. Click Calculate, then click Close.
2. Enter `glidescoremw` in the Create text box.
3. Select the GlideScore property:
  - a. Click Properties.
  - b. Select docking score from the list.
  - c. Click OK.
4. Click the / button.
5. Select the Molecular weight property.

Use the same procedure as in [Step 3](#). The formula is now complete and can be evaluated.
6. Click Execute.

The property is created and the values entered into the table.

#### 9.11.4 Editing Properties

To edit the contents of an individual Project Table cell, click the cell, edit the contents, then press ENTER or click elsewhere in the Project Table. If the cell is not in a selected entry, the entry it is in is selected and all others are deselected.

To set the value of a property to a particular value for the selected entries, click one of the cells, edit the contents, then press CTRL+ENTER. The new value is copied to all selected entries.

You can copy and paste property values using the mouse. To copy a value from the Project Table, click in the cell, then drag over the value you want to copy. To paste the value, click in the cell you want to copy the value to, then middle-click to paste the value into the cell. The value you copy does not need to come from Maestro—you can obtain it from any location.

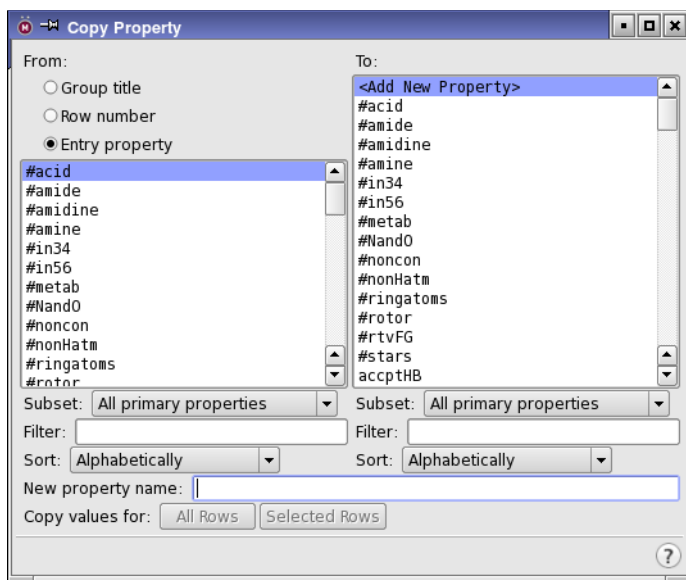


Figure 9.17. The Copy Property panel.

### 9.11.5 Copying Properties

You can copy values from one property to another in the Copy Property panel, which you open by selecting Copy from the Property menu. To copy values, specify the source property (From) and the destination property (To), then click All Rows or Selected Rows to copy the values.

The source and destination properties do not need to have the same data type. The result of the copy operation depends on the characteristics of the data. An entry must always have values for Title, Entry ID, Entry Name, In, Surf, Hyp, Vib, and Selected (the selection state). These property values cannot be deleted. The Entry ID, Surf, Hyp, and Vib properties cannot be overwritten. The Entry Name can only be replaced by a legal entry name. The Title can be made empty, but the property itself cannot be deleted. If the source value is missing or the conversion fails when copying to the In or Selected properties, these properties are set to false.

The following conditions determine what happens when the destination is not one of the special properties:

- If the destination property does not exist, it is created using the data type of the source property and the source data is copied into it.
- If the destination property does exist and is of the same type as the source, the destination property values are replaced.

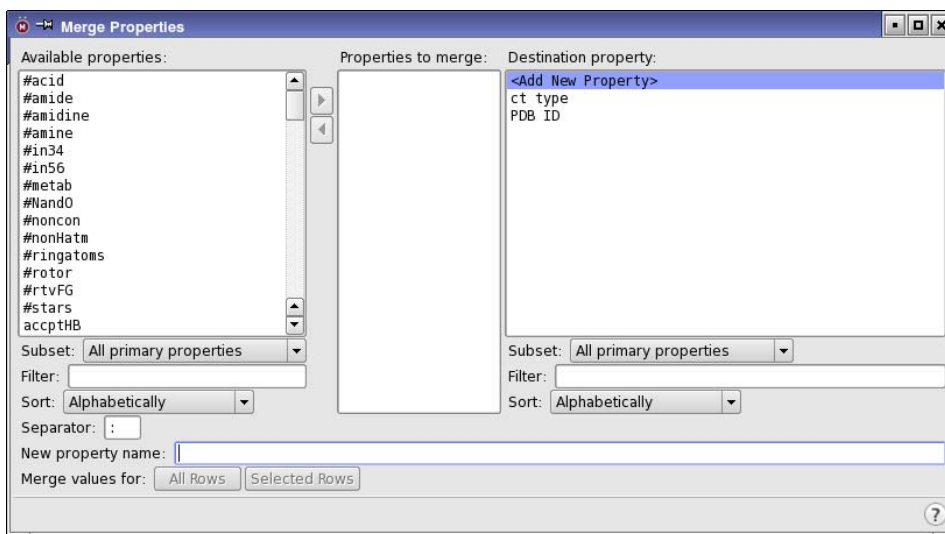
- If the destination property exists and is of a different type, an attempt is made to convert the data type to that of the destination. If the conversion fails, the destination property is deleted. If it succeeds, the converted data replaces the original data.
- If fields in the source property column are empty, the corresponding fields in the destination property column are deleted.

Note that the row number is not a property of the entry. However, it can be copied to a property, by selecting Row in the From section. The From section also has an option for the group title, which you can copy to a property.

See [Section 9.6.6 on page 206](#) for information on copying a range of properties from one entry to other entries.

### 9.11.6 Merging Properties

You can merge the values in one or more property columns into an existing property or a new property in the Merge Properties panel, which you open from the Properties menu. The destination property must be a string property, because the merged property is a list of the selected properties, separated by a delimiter. The source properties can be any kind or property, but they are converted to a string on merging.



**Figure 9.18.** The Merge Properties panel.

**To merge properties:**

1. Select the desired properties from the Available properties list,
2. Click the right arrow to move them to the Properties to merge list.
3. Select the destination property from the Destination property list.
4. (Optional) Enter a separator in the Separator text box.
5. Click All Rows or Selected Rows to perform the merge.

Both property lists have tools that you can use to restrict the list to a given family, filter the list, or sort the list. The order of the source properties in the destination property is the order in which they are sorted in the Available properties list. The merged property is appended to the destination property.

To create a new property, select <Create New Property> in the Destination property list, and enter a name in the New property name text box. The name can include spaces. You can specify a multi-character separator (including spaces) in the Separator text box. Click All Rows or Selected Rows to complete the operation.

### 9.11.7 Setting the Number of Decimals and the Notation for a Real Property

You can change the number of decimal places displayed for a given property, by choosing Property → Columns → Decimal Places or choosing Decimal Places from the Columns button menu on the Property toolbar.



The Set Decimal Places dialog box is displayed, in which you can select one or more properties and set the number of decimal places to display. The default number of decimals is set as a preference—see [Section 14.3.1 on page 341](#) for more information.

You can also select Use E notation, to display the property in exponential notation, e.g. 1.0e-02 instead of fixed- point notation, e.g. 0.01. The properties that you select are shown in the Project Table in E notation, with the specified number of decimal places, when you click Set.

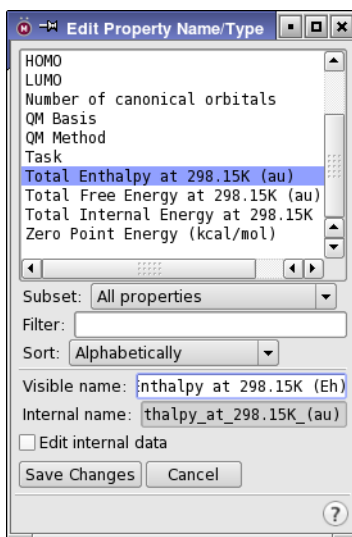


Figure 9.19. The Edit Property Name/Type panel.

### 9.11.8 Renaming Properties

You can rename properties other than the fixed properties, Entry ID, In, Title, Stars, and Entry Name.

To rename a property, choose Property → Columns → Edit Name/Type, or choose Edit Name/Type from the Property shortcut menu or the Columns button menu on the Property toolbar.



You can then edit the name in the Edit Property Name/Type panel.

Properties have a “display name” or “visible name” and an “internal name” (see [Appendix E](#)). You can change both names in this panel. Normally you should not need to edit the internal name, but if you want to change it, select Change internal name. If you change the prefix that specifies the property type, the property values are converted to the new type. If any property value is not converted, a warning is posted so you can revert the change. Otherwise, the values on which the conversion fails are left blank. The name that you choose (either visible or internal) must be unique within the project.

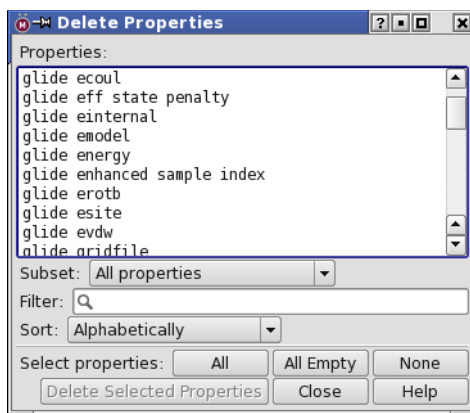


Figure 9.20. The Delete Properties panel.

### 9.11.9 Deleting Properties

You can delete properties other than the fixed properties, Entry ID, In, Title, Stars, and Entry Name.

To delete a single property, right-click on the column heading and choose Delete.

To delete one or more properties, you can choose Property → Delete, which opens the Delete Properties panel. Select the properties in the list and click Delete Selected Properties. You can select multiple properties with shift-click and control-click.

To find the properties you want to delete, you can show a subset of properties, filter the properties, or sort the properties using the property selection tools.

You can select all the properties shown in the list by clicking All. Only the shown properties are selected. You can select the properties for which none of the entries have a value by clicking All Empty. This action selects from all the properties in the project, regardless of the filter.

To clear the selection, click None.

### 9.11.10 Clearing Property Values

You can clear the values of all or selected properties, so that the properties have no value for those entries. To do this, choose Property → Clear Values, select the properties and the target entries (All or Selected) in the Clear Property Values dialog box and click Clear.



### 9.11.11 Showing and Hiding Properties

The Property menu has several choices for selecting the properties that are shown in the Project Table. The choices on the Show submenu are also available from the Show toolbar button.



The Property shortcut menu (displayed when you right-click on a column heading) has several choices for showing and hiding properties—see [Table 9.2 on page 188](#). You can also show and hide properties and property families from the tree view of the properties, which you display by clicking the Tree toolbar button.



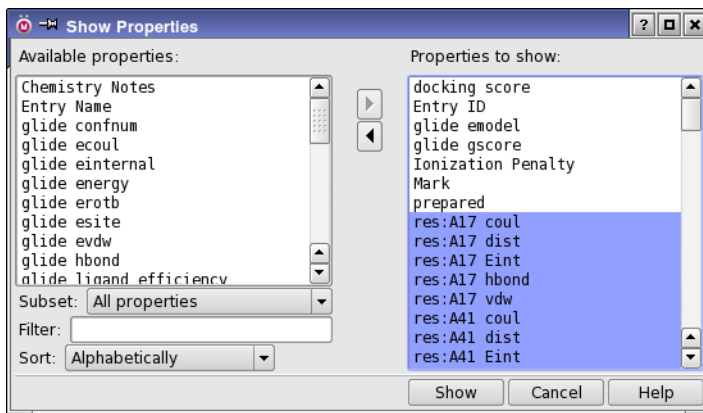
You can set a preference to control whether new properties are automatically added to the display when entries are added to the Project Table, under Project Table – Properties in the Preferences panel—see [Section 14.3.1 on page 341](#).

As well as reducing the amount of data displayed in the Project Table, limiting the displayed properties can be used to limit the properties that are exported to a structure file or a spreadsheet file.

#### 9.11.11.1 Using the Properties Menu

The main ways of selecting the properties using the menu are as follows:

- You can select the properties to show in the Show Property dialog box, which you open by choosing Property → Show → Select. You can select multiple properties in the Available properties list by shift-clicking and control-clicking the list items.



**Figure 9.21.** The Show Properties dialog box.

The list can be restricted to primary properties, a property family or its primary properties, or the shown properties by selecting from the Subset option menu, and it can be filtered by entering the text to match in the Filter text box. This text can include wildcard characters: \* to match any number of characters, ? to match a single character; and it can include character sets enclosed in square brackets, such as [a-z]. You can also sort the list alphabetically or by the order of the Project Table.

When you have selected the desired properties, click the right arrow button or press the RIGHT ARROW key to transfer them to the Properties to show list. If you want to hide properties, select them in the Properties to show list and remove them from the list by clicking the left arrow button or pressing the LEFT ARROW key.

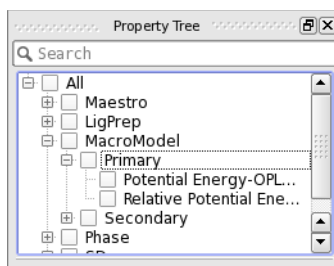
When you have chosen the properties, click Show to change the Project Table display.

- You can display all properties by choosing Property → Show → All.
- You can display only the primary properties by choosing Property → Show → Primary Only.
- If you want to display all the properties or the primary properties for a given family and hide all other properties, you can choose from the Show Only Family submenu of the Properties menu.
- If you want to hide the properties from a given family, you can select the family from the Hide Family submenu of the Property menu.
- You can hide all properties by choosing Property → Show → None.
- The 2D structure can be shown or hidden separately. It has its own item on the Property menu, and a toolbar button.
- You can limit the properties to those for which the selected entries have at least one value defined, by choosing Property → Show → For Selected Entries. This choice removes columns from the display that are empty for the selected entries, allowing you to focus on those that have values.

### 9.11.11.2 Using the Property Tree

The property tree lists all the properties in the Project Table. Each property has a check box that you can use to show or hide the property. The tree is organized by families, with one node for each family, and nodes underneath it for the primary and secondary properties, with properties sorted alphabetically under each node.

To view the properties for a family, click the turner (node). Click the turner again to hide the properties in the tree. If you want to expand or collapse all branches of the tree, right-click on any family (but not on a node) and choose Expand All or Collapse All.



**Figure 9.22. The Property Tree panel.**

The properties that are shown in the tree can be filtered, by entering the text you want to match in the search text box. This text can include wildcard characters: \* to match any number of characters, ? to match a single character; and it can include character sets enclosed in square brackets, such as [a-z]. Filtering is done as you type, and the tree displays only the nodes that contain properties that match the filter. To show the full tree again, click the clear (X) button at the right side of the text box.

To show or hide any property or any group of properties (a property family, or the primary or secondary properties of a family), click the appropriate check box. If a group of properties has some but not all of its properties shown (checked), the check mark is gray, to indicate that the group is incompletely shown.

Since properties can belong to more than one family, when you select a property or a group of properties to be shown, other groups or properties can be selected. For example, selecting the secondary family for Glide also selects the Glide Residue Interactions family, because this family is a subset of Glide secondary properties (see [Figure 9.22](#)).

To scroll a particular property into view in the Project Table, right-click on a property and choose Scroll into View.

### 9.11.12 Creating and Editing Custom Property Families

You can create and edit your own property families in the Manage Custom Property Families panel, which you open from the Property menu. You can create new families, copy families, rename families, edit families, and delete families. You can also redefine the primary property families that are defined for each application. Property family definitions are stored in the file `custom_property_groups` in the profile directory for the current profile, and primary property families are stored in `custom.primary.properties`, in the same location. Thus, they are not tied to a particular project, but are part of your Maestro customization.

Some procedures are given below for creating and editing custom property families. Changes that you make to a property family are applied immediately: there is no confirmation for

changes to the properties included, or for deleting a family. You should therefore take care to make a copy of any family that you do not want to change or delete accidentally. You can also edit the resource files for these families—see [Section 13.5.6 on page 325](#).

The list of available properties can be limited to an existing family, which you can choose from the Subset option menu, or it can be filtered, by entering an expression in the Filter text box. The expression can include wildcard characters: \* to match any number of characters, ? to match a single character; and it can include character sets enclosed in square brackets, such as [a-z]. The beginning and end of the expression have implicit \* wildcard characters.

### To create a new property family from scratch:

1. Click New.

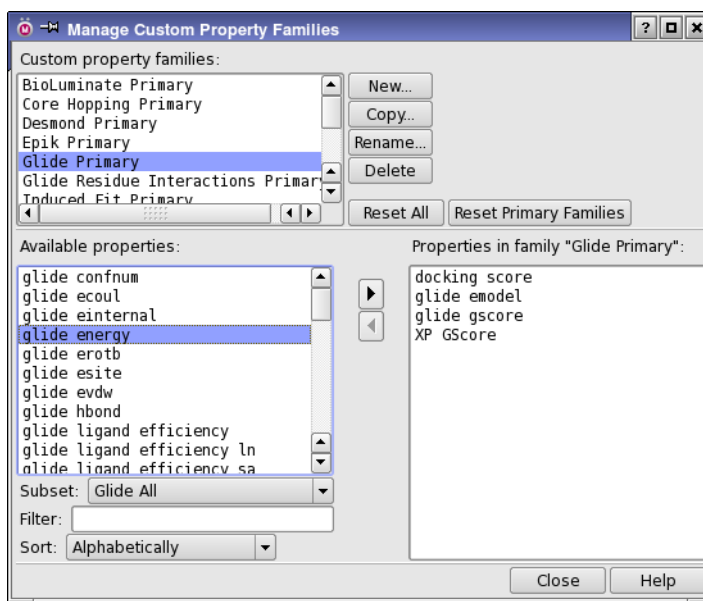
The New Family dialog box opens.

2. Enter a name for the property family and click OK.

The dialog box closes and the family name is shown in the Custom property families list.

3. Select the properties that you want to add to the family in the Available properties list.

To select the properties, you can use shift-click and control-click as usual; you can choose a subset of the properties from the Subset option menu; and you can filter them by entering an expression in the Filter text box.



**Figure 9.23.** The Manage Custom Property Families panel.

4. Click the arrow button that points to the right (the upper one) or press the RIGHT ARROW key.

The properties you selected are transferred to the Properties in family list.

5. Repeat the selection and transfer steps until you have all the properties you want in the family.

**To create a new property family from an existing family:**

1. Select the existing family in the Custom property families list.
2. Click Copy.

The Copy Family dialog box opens.

3. Enter a name for the property family and click OK.

The dialog box closes and the name is displayed in the Custom property families list.

4. Select the properties that you want to add to the family in the Available properties list, and click the right arrow button or press the RIGHT ARROW key.
5. Select the properties that you want to remove from the family in the Properties in family list, and click the left arrow button or press the LEFT ARROW key.

**To change an existing property family:**

1. Select the existing family in the Custom property families list.
2. Select the properties that you want to add to the family in the Available properties list, and click the right arrow button.
3. Select the properties that you want to remove from the family in the Properties in family list and click the left arrow button or press the LEFT ARROW key.

Note that the changes to the family are immediate: there is no confirmation.

**To delete a property family:**

1. Choose the family in the Custom property families list.
2. Click Delete.

The family is deleted immediately.

**To delete all custom property families:**

- Click Reset All.

All families are deleted, and any customization of the primary families is reverted.

**To restore the primary property families to their defaults:**

- Click Reset Primary Families.

You can also customize the primary property families from the Tree view of the properties, by dragging properties between the primary and secondary sets within a family. To display the tree view, choose Property → Tree or click the Tree button.



### 9.11.13 Coloring Table Cells By Property Value

You can define how the cells in property columns are colored, using the numerical values of the property. The property must have real or integer values. The properties for which a cell color scheme is applied can be selected, and the color schemes for the cells can be set up, modified, applied, and saved as preferences, in the Color By Property dialog box. To open this dialog box, choose Entry → Color → By Entry Property, or choose By Entry Property from the Color toolbar button.



**To apply a color scheme to a property column in the Project Table:**

1. Select the property in the Available properties list.

You can restrict the range of properties shown with the Subset option menu, filter them by entering a string in the Filter text box that the property name must include, or sort them by choosing a sort option.

2. Click Add.

The property is transferred to the Colored properties list, selected, and is listed in the Property text box. The range of property values is reported below the Property text box. If the property has previously had color settings, these settings are restored. Otherwise, standard default values are set.

3. Select the desired options for coloring the property, and set the value thresholds and choose the colors (see below).
4. Click Apply to apply the scheme and continue on to color another property, or click OK to apply the scheme and close the dialog box.

**To remove a color scheme:**

1. Select the property in the Colored properties list.
2. Click Remove.

The property is transferred to the Available properties list. The coloring is turned off, but the scheme is still available if you decide to reapply coloring.

**To change a color:**

1. Click the color button.

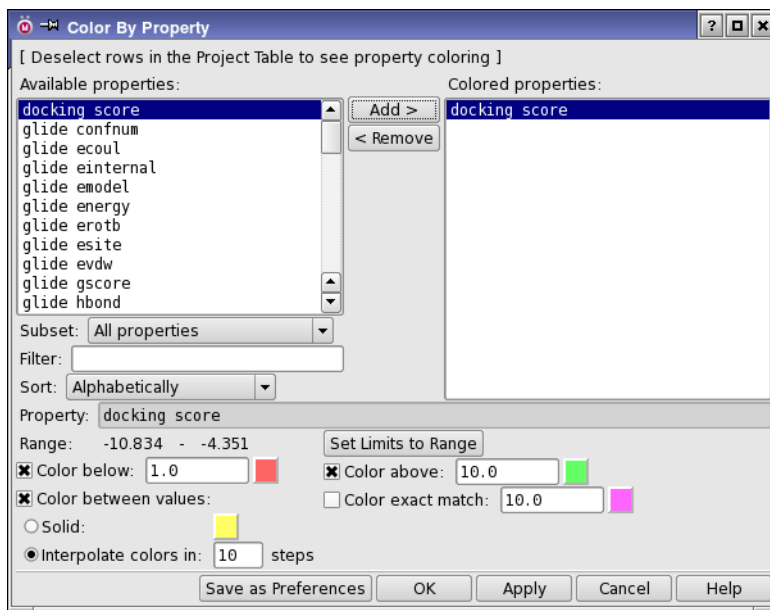
A standard color selector opens.

2. Pick the color or specify its numerical values (HSV or RGB).
3. Click OK.

The new color is displayed on the color button.

The color scheme is defined by the options in the lower part of the panel, with their controls.

- Color below—Select this option to color property values that are below the specified threshold. The threshold is a strict inequality ( $value < threshold$ ) You can enter the threshold in the text box.



**Figure 9.24.** The Color By Property dialog box.

- **Color above**—Select this option to color property values that are above the specified threshold. The threshold is a strict inequality (*value > threshold*) You can enter the threshold in the text box.
- **Color between**—Select this option to color property values that are between the Color below and Color above thresholds. There are two options:
  - **Solid**: Use a single color between the two thresholds.
  - **Interpolate colors in N steps**: Interpolate the colors between the Color below and Color above colors in the given number of steps. The range of values between the two thresholds is partitioned into steps of the same size.
- **Color exact match**—Select this option to color property values that are equal to the specified value (*value = target*) You can enter the target value in the text box.

The range of property values for the selected property is reported above these options. You can set the limits in the Color below and Color above text boxes to the minimum and maximum values of the property by clicking **Set Limits to Range**.

If you want to save the property color schemes for use in other projects, click **Save as Preferences** when you have finished defining the color schemes. The schemes are saved in your [Maestro user resources directory](#). These preferences are read and applied to properties in any project, not just the current project, and are used as the default colors. The property color schemes are stored in the project by default, and are used whenever the project is opened.

### 9.11.14 Moving, Reordering, and Resizing Property Columns

There are several ways of moving individual property columns and multiple columns.

You can move and resize individual columns in the Project Table with the mouse. Dragging a column border resizes the column. Dragging the column heading moves the column. You can only move columns that are in the scrollable area.

More options for moving an individual column are available from the Property shortcut menu, which is displayed when you right-click in a column heading. The following options are available from the **Move To** submenu:

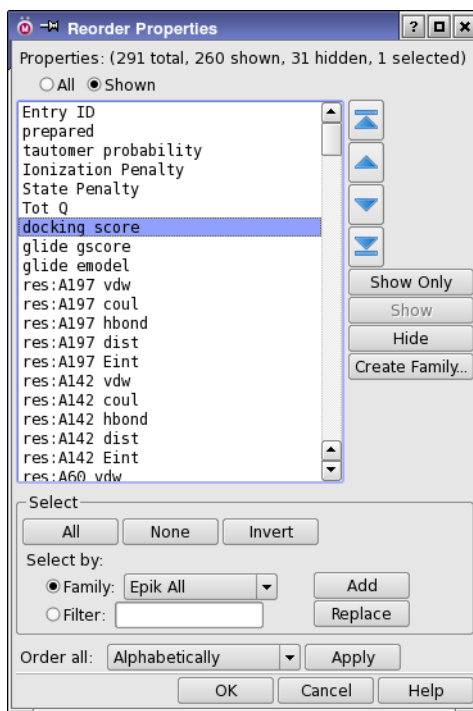
- **First**—Move the property to the first (leftmost) position in the scrolling area of the table.
- **Before**—Move the property to the position before the property that you choose in the property selector that opens.
- **Left**—Move the property one place to the left.
- **Right**—Move the property one place to the right.



- **After**—Move the property to the position after the property that you choose in the property selector that opens.
- **Last**—Move the property to the last (rightmost) position in the scrolling area of the table.
- **Fixed Area**—Move the property to the fixed area of the table. The property is added after the standard fixed properties, and cannot be moved to a position to the left of any of these properties.
- **Scrolling Area**—Move the property to the scrolling area of the table. This can only be done for properties that you moved from the scrolling area. The property is placed in the first position of the scrolling area.

If you want to rearrange multiple columns, use the Reorder Properties dialog box, which you open by choosing Property → Reorder. In addition to reordering the properties, you can select properties to show or hide, and create new property families. Properties can be reordered by selecting them in the Properties list, and moving them to their desired new location in the list.

To choose the scope of reordering, select All or Shown. The Properties list is updated to reflect the choice, and the count of properties at the top of the panel is updated. If you display all



**Figure 9.25.** The Reorder Properties dialog box.

properties, the properties that are currently hidden are listed in italics. You can show or hide properties in the list by selecting them and clicking Show Only, Show, or Hide. The font is changed to reflect the new status. If Shown is selected, and you click Hide, the properties are hidden. The visibility of the properties in the Project Table is not changed until you click OK.

You can select properties in the list with the usual click, shift-click and control-click in the list, or with the tools in the Select section of the panel. In this section, you can select by family or by using a filter, then click Add to add to the selection or click Replace to replace the selection.

To move properties in the list, you can drag them to the new location, or use the four arrow buttons to the right of the list. If the list does not display hidden properties, the moved properties are placed above any hidden properties that are above the insertion point.

If you want to create a custom family, you can select properties in the list, then click Create Family. When you enter a name and click OK in the Create Custom Property Family dialog box, the family is created and added to the Family option menu. It can then be used for selection of properties.

Properties can also be reordered alphabetically or by family. To do so, choose the appropriate option from the Order all option menu, and click Apply. When properties are ordered by family, the families are arranged alphabetically, but the order of the properties within the families is not changed. Properties that are not in families or in the scope of the option chosen are placed at the end of the list, in their current order.

You can resize all columns to fit the width of the data, to fit the width of the data and the heading, or to a fixed width by choosing the appropriate item from the Columns button menu or the Columns submenu of the Table menu.

### 9.11.15 Exporting and Importing Data

Maestro does not provide full spreadsheet capabilities. However, you can export data to a spreadsheet file, operate on the properties, and re-import the modified data. These capabilities are available from the Import and Export submenus of the Table menu, and are discussed in detail in [Section 3.3 on page 57](#) and [Section 3.4 on page 58](#). You can also export data along with structures to Canvas—see [Section 3.5 on page 60](#).

# Tools

Maestro is equipped with tools for investigating and changing the properties of structures in the Workspace. While some of these tools, such as plotting ([Chapter 11](#)) are discussed elsewhere, most of the tools are discussed here. The tools are available on the Tools menu.

## 10.1 Displaying Markers

Maestro uses markers to mark atom selections in the Workspace. These markers provide visual confirmation that atoms have been successfully selected, or that an analysis task or operation has been performed.

For most operations, you can choose whether or not to display markers. To display the markers for a particular operation, select **Show markers** or **Markers** in the panel used to perform the operation. When you are no longer using a property represented by a set of markers, you can hide the markers so that the Workspace does not become cluttered. The atom sets remain defined, so that you can redisplay the markers later.

Most panels display markers by default, and hide their associated markers when you close the panel. The exception is measurement markers, which are displayed even if the **Measurements** panel is hidden. You must delete these markers explicitly.

The color of some markers can be changed. If there is a colored button or a color patch and an **Edit** button next to the **Show markers** or **Markers** option, you can click the button and select a color for the marker in the color selector that opens. The color is shown in the color patch.

## 10.2 Displaying Measurements in the Workspace

The **Measurements** panel (see [Figure 10.1 on page 248](#)) provides tools to determine the geometric relationships between atoms in the Workspace, and other geometry-dependent properties, and display them in the Workspace. These tools are contained in four tabs—**Distances**, **Angles**, **Dihedrals**, and **1H NMR Coupling**.

The **Non-Bonded Interactions** panel (see [Figure 10.2 on page 249](#)) provides tools for displaying hydrogen bonds, halogen bonds, contacts, and pi interactions between atoms that are not directly bonded. Nonbonded interactions are considered measurements even though no measurement is explicitly made, because there are specific value ranges of atom distances and angles that must be satisfied.

To open the Measurements panel at a particular tab, choose the tab name from the Measurements submenu of the Tools menu. This panel is a dockable panel. Measurements can also be made from the Labels toolbar. To open the Non-Bonded Interactions panel, use the Tools menu.

Settings that affect the display of measurements and nonbonded interactions can be made in the Preferences panel (see [Section 14.7 on page 357](#) and [Section 14.8 on page 357](#)).

## 10.2.1 Measuring Distances, Angles, Dihedrals, and NMR Coupling

The controls for Distances, Angles, Dihedrals, and  $^1\text{H}$  NMR Coupling are very similar, as are the actual measurement procedures for these quantities. To measure a distance, you need to specify only two atoms or one bond, for an angle you must specify three atoms or two bonds, and for dihedrals you must specify four atoms or three bonds.

To select atoms for measurement, select the Add mode, then choose Atoms or Bonds from the Pick option menu in the Define atoms for measurement section, and select the atoms or bonds in the Workspace. When you have selected the requisite number of atoms, the measurement is made and entered into the measurement list. If Markers is selected, a dashed line indicating the atom locations and the numerical value obtained from the measurement is displayed in the Workspace. Distances are marked in purple, angles in green, and dihedrals in red, but you can change the color by clicking Edit and choosing a new color in the color selector.

Once you have defined atoms for a measurement, those atoms remain defined until you delete the atom set or remove the structure from the Workspace. If you only temporarily want to undisplay the results of your measurements, deselect Markers. However, if you no longer need the measurement value itself, you can remove it by selecting the corresponding list item and clicking Delete. To delete all of the atom sets currently defined for a particular type of measurement, click Delete All.

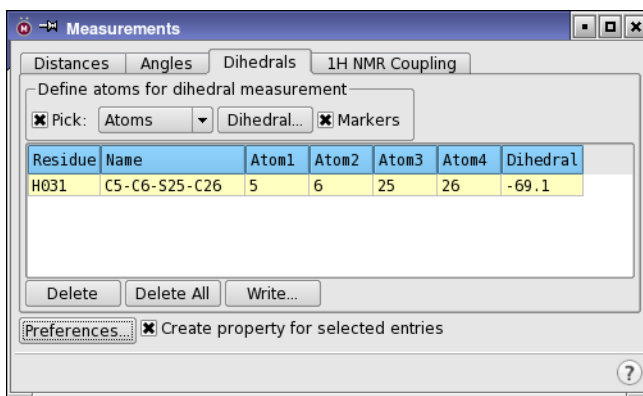


Figure 10.1. The Dihedrals tab of the Measurements panel.

Distances to surfaces can also be measured, by choosing Atoms & Surfaces from the Pick menu in the Distances tab. The distance is given to the point on the surface where you click.

You can make measurements with the Measure toolbar button.



To make a measurement, choose Distance, Angle, Dihedral, or 1H NMR Coupling from the button menu, then click the atoms in the Workspace. The measurement is made, and any options that are set in the Measurements panel are applied: for example, if Create property for selected entries is selected, the property is created.

## 10.2.2 Displaying Nonbonded Interactions

Nonbonded interactions, such as hydrogen bonds, halogen bonds, contacts, pi-pi stacking interactions, and pi-cation interactions, can be displayed using the Non-Bonded Interactions panel, which you can open with any of three items on the tools menu: H-Bonds and Halogen Bonds, Contacts, and Pi Interactions. (Hydrogen and halogen “bonds” are considered nonbonded interactions, as they are not covalent bonds.)

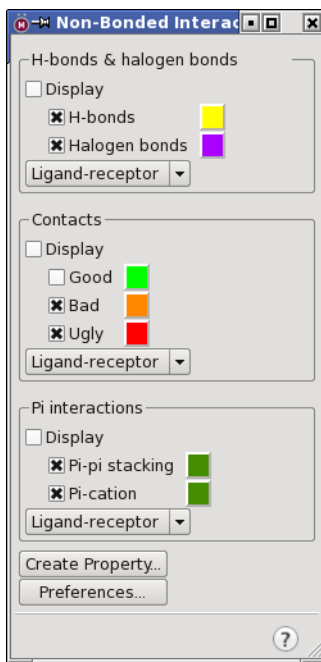


Figure 10.2. The Non-Bonded Interactions panel.

To mark any of the three main types of interactions in the Workspace, select the Display option in the section for that interaction type. To choose which interactions of the three types you want to display, select the option for that interaction. The color of the markers can be changed by clicking the color button and choosing a new color in the color selector that opens.

The criteria for defining hydrogen bonds or contacts can be changed in the Preferences panel—see [Section 14.8.1 on page 357](#).

All nonbonded interactions that are found within or between the specified atom sets are displayed. You can choose these atom sets from the option menu in the section for each interaction type. The predefined sets are Ligand-receptor, which displays interactions between any ligand and any receptor in the Workspace; Intra-ligand, which displays interactions within any ligand in the Workspace, and All, which displays all interactions for all the Workspace atoms.

You can also choose Other to define the atom sets for the interactions. The Edit *interaction* Definition dialog box opens, and an Edit button is placed next to the option menu in the Non-Bonded Interactions panel. To define atom sets, use the atom selection tools—see [Section 6.3 on page 121](#) for a description of these tools. If you define only Atom set 1, the interactions are displayed within that set. If you define both Atom set 1 and Atom set 2, the interactions are displayed between the two sets.

You can also display interactions from the Measurements toolbar. There are three buttons, one for each interaction type. The buttons have menus that offer the same choices for display and atom set definition as in the panel (and are kept in sync).



### 10.2.3 Displaying H-H NMR Coupling Constants

NMR spin-spin coupling constants can be estimated for vicinal hydrogen atoms using a modified Karplus-type calculation (Haasnoot et al. *Tetrahedron* **1980**, *36*, 2783). To display the estimated coupling constants, you must select two hydrogen atoms that are bonded to two carbon atoms, and these carbon atoms must be bonded to each other. The controls are the same as for distance measurements. You can also display coupling constants from the toolbar, using the Measurements button.

### 10.2.4 Storing the Results of Measurements

You can include measurements as properties in the Project Table, and you can export measurements to a tab-delimited or comma-delimited file.

To create properties for measurements, select **Create property** for selected entries before you define the measurements. The properties are added to the selected entries in the Project Table. Each distance, angle, or dihedral becomes a separate property, and is labeled with the name Distance, Angle, or Dihedral and the atom numbers that define the geometric quantity.

To create properties for nonbonded interactions, click **Create Property** in the Non-Bonded Interactions panel. A dialog box opens, in which you can choose the type of interaction to create properties for. The properties are the number of interactions of each type.

Each tab in the Measurements panel has a **Write** button, which allows you to write a file containing the measurements. The **Write** button opens a panel in which you can specify a delimiter for the file and a file name. If you specify a name or a relative path in the File text box, the file is written relative to the Maestro working directory. If you click **Write To**, a dialog box is displayed in which you can navigate to the desired directory and select a file or enter a file name.

The file consists of a header line, a blank line, then lines containing the data, one line for each measurement. The data written is as follows:

- For distances and angles, the atom numbers are listed, followed by the measurement value.
- For dihedrals, the residue number is listed first, then a label that consists of the element and atom number for each atom, separated by hyphens, then the atom numbers, then the dihedral angle.
- For hydrogen bonds, the hydrogen atom is listed first, as *element(atom#)*, followed by the acceptor atom in the same format, then the A-H distance, the D-H-A (donor heavy atom–donor hydrogen–acceptor) angle, and the H-A-B (donor hydrogen–acceptor–atom attached to the acceptor) angle. The header also lists the current criteria for H-bond acceptance.
- For contacts, the two atoms are listed first in the format *element(atom#)*, followed by the distance, the contact cutoff ratio, and the type (Good, Bad, or Ugly).

### 10.2.5 Defining Dummy Atoms for Measurements

Dummy atoms can be useful for making measurements. For example, you can measure the distance between the centroids of two ring systems by placing dummy atoms at the centroids. You can place dummy atoms in two ways:

1. Use the **Centroid** panel to define a centroid atom.

A dummy atom is placed at the mean position of the picked atoms.

2. Use the Draw button on the Build toolbar to place an atom in the Workspace, then retype it with the appropriate MacroModel atom type.

Several kinds of dummy atoms are defined in the Atom Type (MacroModel) list in the Atom Properties tab of the Build panel. If you attach the dummy atom to your structure, you can adjust its position using the Adjust panel.

## 10.2.6 Positioning and Formatting Measurement Labels

The formatting and the position of the text label that displays the measurement values can be changed. The number of decimal places, the color, and the font used are set as preferences, in the Measurements tab of the Preferences panel—see [Section 14.7 on page 357](#). The font size can also be adjusted with the font buttons on the Labels toolbar.



The position of each label can be adjusted by dragging the label to its desired location.

## 10.3 Superimposing and Aligning Structures

If you want to determine the similarity of structures such as a set of conformers or a family of ligands docked by Glide, you can use two tools on the Tools menu: Superposition, and Flexible Ligand Alignment. There is also a Phase command-line utility, `rmsdcalc`, that can calculate and minimize the RMSD of a set of structures with respect to a reference structure.

Protein structures can be aligned with the protein structure alignment program, which has two panels for performing the alignment: Align Binding Sites, and Protein Structure Alignment. The second of these is the more general tool.

### 10.3.1 The Superposition Panel

You can use the Superposition panel to rigidly superimpose a set of structures and evaluate the differences in the atom positions. Each structure must be in a separate project entry. To open the Superposition panel, choose Superposition from the Tools menu.

The superposition scheme works by aligning the first selected atom in each structure, then attempting to align the second selected atom, and so on. The atoms are aligned to the first entry in the Project Table that is being used in the superposition (the *reference* entry). After superimposing atoms, the results of the operation are displayed in the RMSD text box near the bottom of the panel. The results include the molecule numbers, the RMS deviation of the atoms from those of the first structure, and the maximum difference between superimposed atom positions. The results accumulate as you perform superpositions, so you can click Clear to clear them.



There are two choices for the entries that are used for the superposition: the included entries (those in the Workspace), or the selected entries (those selected in the Project table). This choice is available under Entries to superimpose. If you choose Selected entries, you must have at least one entry displayed in the Workspace to be able to pick atoms for superposition.

There are four choices for the method of superposition, displayed in four tabs:

- **Atom pairs**—To compare two structures, you can select the atoms to superimpose in each structure in pairs. To define the atom pairs, select Pick atom pairs, then pick the atom pairs. You must pick one atom from each entry, and you must pick the first atom from the same entry each time. The atom pairs are displayed in the Superimpose by atom pairs text box as you pick them. If Show markers is selected, the atom pairs are connected by dashed lines. Once you have picked the first pair, Superimpose Atom Pairs, Delete, and Delete All are activated. If you need to delete a pair, select the pair in the list and click Delete. To delete all pairs, click Delete All. After all the atom pairs are selected, click Superimpose Atom Pairs to superimpose the two structures.
- **ASL**—To superimpose the displayed or selected structures based on all the atoms in the structures, click All in the ASL tab. The superposition is done using the atom numbers. This option is useful if each entry has the same number of atoms and is numbered the

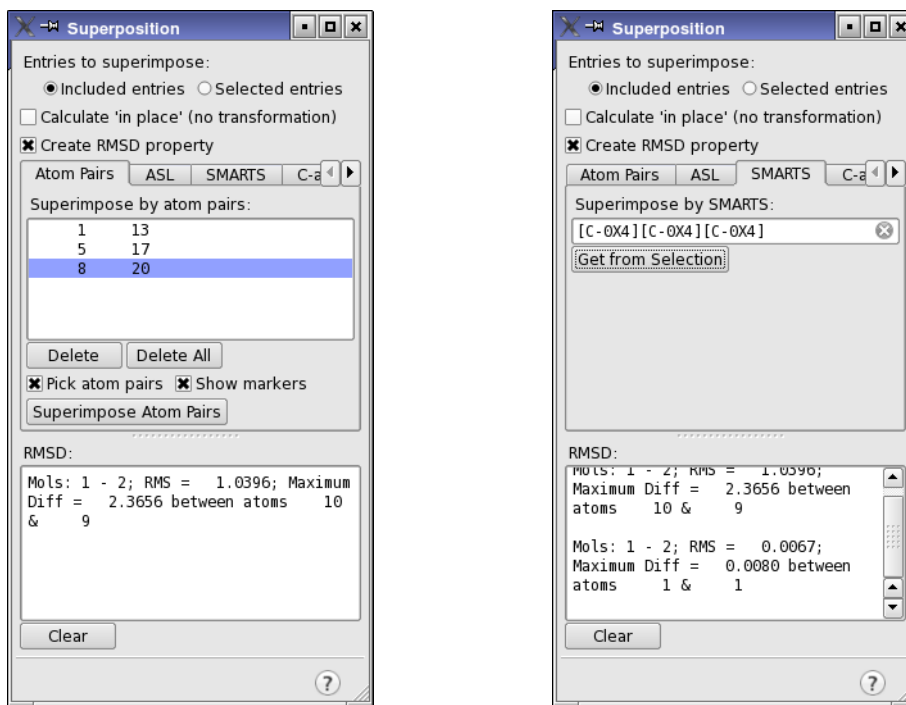


Figure 10.3. The Superposition panel, showing the Atom Pairs and the SMARTS tabs.

same way, which usually requires that the entries be conformers. When you click All, the superposition is done with the maximum use of local symmetry. You can also type `all` in the text box, or make a selection from the Atom Selection button, but the superposition does not use symmetry in this case.

If the structures you want to compare are not conformers, or if you only want to compare part of the structure, you can select the atoms to superimpose by making a selection in the Workspace and clicking Selection, or by clicking Select and using the Atom Selection dialog box to select the atoms, or by entering the ASL expression in the text box. For example, to use only carbon atoms for the superposition operation, type `atom.e C` and press ENTER. For more information on the Atom Specification Language, see the *Maestro Command Reference Manual*.

- **SMARTS**—To superimpose atoms defined by a SMARTS pattern, you can enter the pattern in the Superimpose by SMARTS text box, or you can create a SMARTS pattern from the atoms that are selected in the Workspace. This method is useful if you want to superimpose structures in which the atom numbering of key parts of the molecule is different, such as conformers that do not have the same atom numbering.

To select the Workspace atoms and create a SMARTS pattern from them, first use the Select atoms toolbar button to select the atoms. Once you have selected the desired atoms, click Get From Selection. The SMARTS pattern corresponding to the selected atoms is entered in the Superimpose by SMARTS text box. You can set preferences for some of the notational elements in the SMARTS pattern—see [Section 14.14 on page 375](#).

- **C-alpha**—To superimpose proteins by their alpha carbon atoms, click Choose to choose the entry that you want to superimpose to, then click Superimpose. The entry you choose must be one of the entries you are superimposing. This tab simply uses a particular choice of ASL to do the superposition, but provides a convenient way of superimposing proteins without regard to residue identity. It is mainly useful for similar proteins, such as mutants of a parent protein. See [Section 10.3.4 on page 256](#) for more protein alignment tools.

The default action when superimposing structures is to apply a transformation to the entries, then calculate the RMS difference in coordinates. If you want to preserve the coordinates of the superimposed structures, select Calculate 'in place' (no transformation). The RMS difference is then calculated without moving the structures. This is a convenient way of obtaining RMS differences for ligand poses in a receptor, for example.

If you do not use the calculate in place option, you can separate the superimposed entries by choosing Edit → Undo.

You can store the RMS deviation as a property for each entry that was superimposed. To create a property, select Create RMSD property before you perform the superposition. The property is labeled RMSD *entry-ID* or RMSD In Place *entry-ID*, depending on how you performed the

superposition. The reference entry has a value of zero for this property. The reference entry ID is used for *entry-ID* in the label. If you change the details of the superposition but do not change the reference entry, the property values are replaced. You can always rename the property if you want to keep it and perform other superpositions with the same reference entry. See [Section 9.11.8 on page 235](#) for information on renaming properties.

### 10.3.2 The Flexible Ligand Alignment Panel

The Flexible Ligand Alignment panel allows you to perform a flexible alignment of the entries that are selected in the Project Table, in which dihedral angles are varied but bond lengths and angles are kept fixed. To open the Flexible Ligand Alignment panel, choose Tools → Flexible Ligand Alignment.

The first selected entry is used as a template, and is kept as is. The remaining ligands are then aligned to this template. The conformation of the structure changes, so you should ensure that you copy the original structures if you want to keep them.

There are two methods you can choose for the alignment:

- Flexible shape-based alignment—a ligand torsional search is performed with ConfGen (see the ConfGen User Manual for details). The conformers generated by ConfGen are then aligned in turn to the reference ligand, and the conformer that has the best overlap with the reference ligand is chosen.
- Common scaffold alignment—common scaffolds among the ligands are detected, and the ligands are aligned on the scaffold, with conformational variation of the side chains. This option requires a Phase license, as the alignment is done with the `phase_align_core` utility. Ligands with no scaffold in common with the template are not aligned.

The structures must include hydrogens—implicit hydrogens are not permitted—and should be well-minimized structures.

To align the ligands click Align Selected Entries. The alignment can take 1–2 seconds per entry.

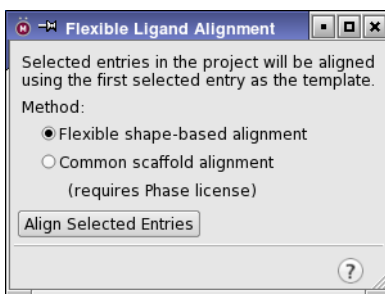


Figure 10.4. The Flexible Ligand Alignment panel.

For more options to align the molecules, including the use of a flexible template, you can use the `flex_align` utility, which is distributed as part of Phase (and requires a Phase license). See [Section C.9](#) of the *Phase User Manual* for details.

### 10.3.3 Aligning Centers of Mass

If you want to align the centers of mass of several structures (which are in separate entries), you can do so as follows:

1. Include the entries in the Workspace
2. Select the atoms in each structure to use for calculating the center of mass.
3. Right-click in the Workspace and choose **Align Centers of Mass**.

The structures are translated so that the centers of mass coincide with that of the reference structure, which is the entry with the lowest row number in the Project Table. There is no rotation of the structures to align the principal axes.

### 10.3.4 Aligning Proteins

If you want to bring two or more proteins into a common frame of reference by structurally aligning (superimposing) them, you can use the **Protein Structure Alignment** panel or the **Align Binding Sites** panel, both of which you open from the Tools menu. For information on these panels, see [Chapter 7](#) of the *Prime User Manual* or the online help for the panel.

## 10.4 Using Atom Sets

Sets are groups of atoms that can be used in a variety of Maestro operations. The Sets panel is used to define these atom groups for subsequent operations, and can be used to save and read set definitions. Set definitions are automatically saved with the current project and are included when the project is copied or merged with another project.

To open the Sets panel, choose **Tools** → **Sets**. This panel is dockable.

### 10.4.1 Creating and Deleting Sets

To create a new set, click the **New** button. In the dialog box that appears, enter a name for the set and click **OK**. This name is used to identify the set in later operations. The name is added to the list at the top of the Sets panel.

To delete a set, select the set name in the set list and click **Delete**.

## 10.4.2 Selecting Atoms for a Set

To define the atoms that make up a set, select the set from the set list, then use the tools in the Atoms For Set section to select the atoms. You can pick the atoms using the picking tools, enter an ASL expression in the text box, or click the Atom Selection button to select predefined atom groups or open the Atom Selection dialog box. The Atom Selection dialog box has a Create Set button, which you can use to create a set at any time, not just from the Sets panel. You can also select sets in the Atom Selection dialog box and perform logical operations on them to construct a new set.

If you select Markers, the atoms in the set are marked with green markers. If the markers obscure part of the structure that you want to see, you can move them slightly by selecting Apply marker offset. This option is selected by default.

For more information on ASL, see the *Maestro Command Reference Manual*, Chapter 3. For more information on the Atom Selection dialog box, see [Section 6.5 on page 125](#).

## 10.4.3 Reading and Writing Sets

You can save set definitions to disk for use with multiple projects. Click Write to open the Write Set Files panel. In this panel, navigate to the directory in which you wish to save the set definitions, and enter a name for your sets definition file. The extension `.set` is automatically appended to the file name. Click Write to save the file and dismiss the panel.

To read an existing sets definition file, click Read in the Sets panel, then navigate to the desired directory and select the file in the Read Set Files panel, and click Read.

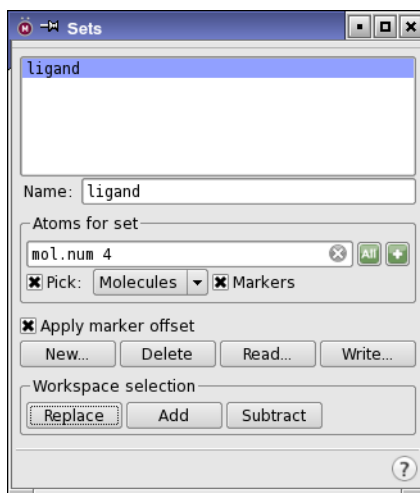


Figure 10.5. The Sets panel.

## 10.4.4 Selecting Atoms in the Workspace that Match a Set

You can use the sets that you have defined to select atoms in the Workspace. Select the set you want to apply to the Workspace in the sets list, then click one of the buttons in the Workspace selection section:

- **Replace**—Replace the current Workspace selection with the selection of atoms that match the set.
- **Add**—Add the atoms that match the current set to the Workspace selection.
- **Subtract**—Remove any atoms that match the current set from the Workspace selection.

## 10.5 Ligand Analysis Tools

The Tools menu contains several ligand-related tools. This section describes two tools that can be used to analyze ligands in terms of a scaffold, to which side chains have been added, and examine properties of the ligands based on this analysis.

### 10.5.1 R-Group Analysis

The R-group analysis tool analyzes properties of a set of ligands in terms of a common scaffold, or core, and its side chains, or attachments, which are the R groups. The analysis is represented in terms of the set of R groups at each attachment site. A full description of this tool is given in the document *R-Group Analysis*.

### 10.5.2 Scaffold Decomposition

One way of finding common structural features in a set of structures is to decompose each structure into a set of scaffolds, then make a list for each scaffold of the structures that contain that scaffold. You can perform this scaffold decomposition in the Scaffold Decomposition panel, which you open from the Tools menu.

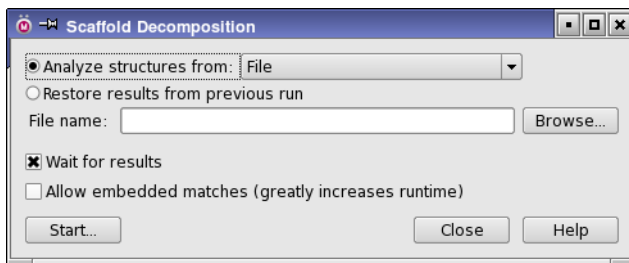


Figure 10.6. The Scaffold Decomposition panel.

To run a scaffold decomposition, select **Analyze structures** from and choose the source of structures from the option menu. If you choose a file, specify the file name or click **Browse** to locate the file.

The decomposition is done by first removing side chains from all ring systems, to define the largest scaffold in the structure. This structure is then split into all possible subscaffolds by breaking bonds and removing linkers between rings, other than those in fused rings. The list of scaffolds is collated, and then for each scaffold, the structures that contain that scaffold are located and added to a list.

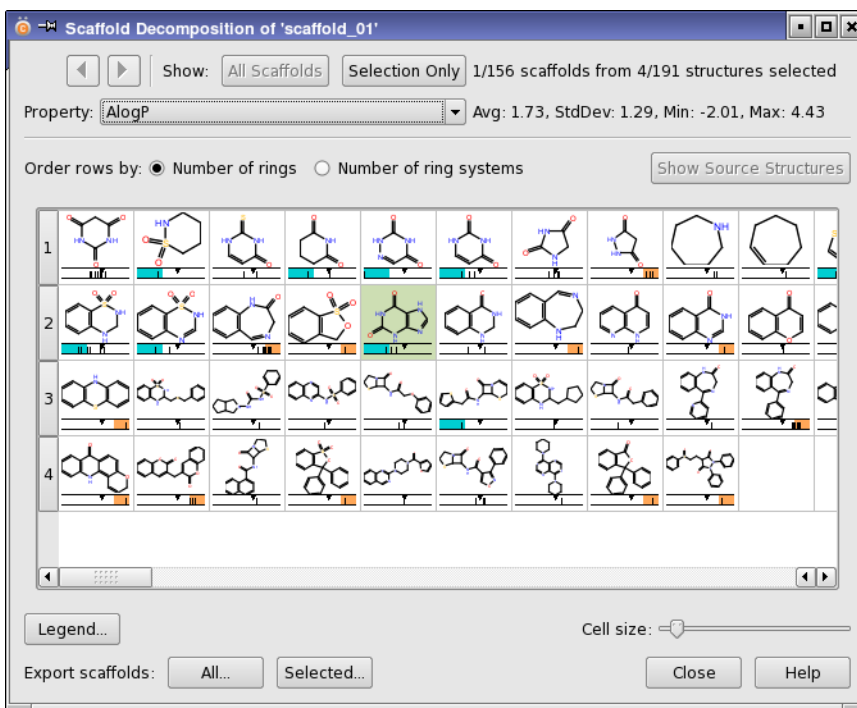
When finding the structures that contain a scaffold, you can choose to match scaffolds to a fused ring system in a structure that contains the scaffold. This is called an “embedded match”, and you can allow them by selecting **Allow embedded matches**. For example, if the list of scaffolds contains imidazole and benzimidazole, a structure that contains benzimidazole is included in the list of structures that contain the imidazole scaffold, if embedded matches are allowed. Identifying embedded matches takes substantially more time than not doing so.

If you want to view the results as soon as the job finishes, select **Wait for results**. Otherwise, you can view the results at a later time by selecting **Restore results from previous run**, supplying the file name for that run, *jobname\_scaffolds.dat*, and clicking **Restore**. In either case, the **Scaffold Decomposition of *jobname*** panel opens.

The **Scaffold Decomposition of *jobname*** panel shows the 2D structures of the scaffolds in a table. The scaffolds can be classified by the number of rings in each scaffold, or by the number of ring systems. The scaffolds for a given classification are shown on the same table row. You can select scaffolds in the table, and limit the display to show only those scaffolds. Each time you limit the display (or remove the limits), that view of the table is stored, and you can use the arrow buttons to step through these views. If you want to see all the subscaffolds or superscaffolds of a particular scaffold, right-click in its table cell and choose the appropriate command.

The table also shows the property distribution of the structures that contain each scaffold, for a property that you can choose from the **Property** option menu. The average, standard deviation, minimum, and maximum values of the property are displayed to the right of the option menu. The property distribution is displayed for each scaffold as a “stick spectrum” in a bar that represents the full range of the property. For each structure there is a vertical line at the property value for that structure. The average property value is marked, and the region outside one standard deviation from the average is colored if it contains vertical lines for property values.

You can export the scaffolds to a structure file. The scaffolds are stored internally as canonical SMILES strings, so if you choose **Maestro** or **SD** format for the file, they are exported as 2D structures without hydrogens, except where the hydrogens are part of the SMILES string.



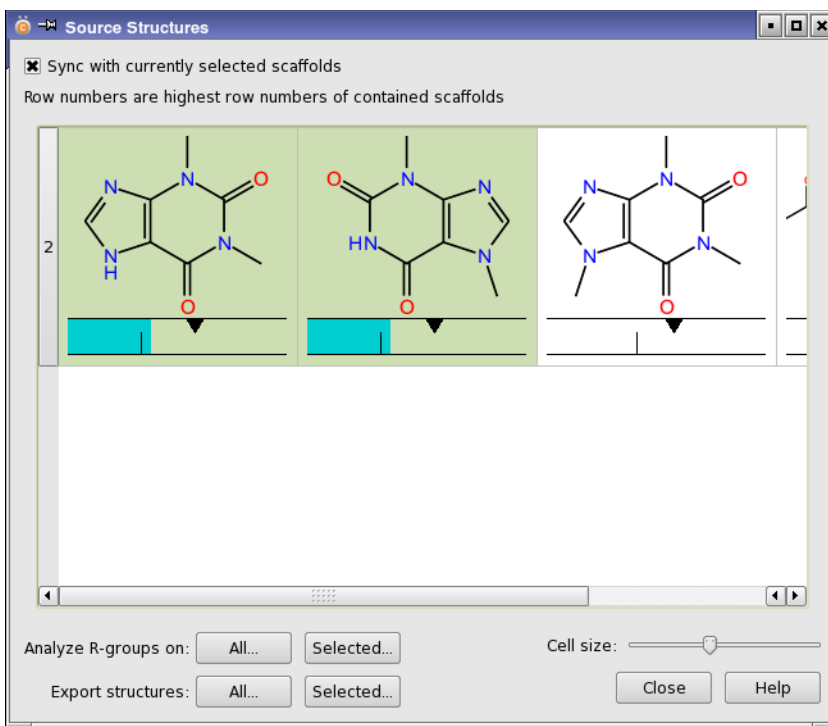
**Figure 10.7. The Scaffold Decomposition of jobname panel.**

If you want to see the source structures for a set of scaffolds, select them in the table and click Show Source Structures. The Source Structures panel opens, and displays the structures for those scaffolds, arranged in rows with the same classification as for the scaffolds, and including the property distribution display. You can export selected structures or all structures to a file. You can run an R-group analysis on the selected structures or on all structures in the panel. If the structures have more than one scaffold in common, you are prompted to choose the scaffold you want to use for R-group analysis.

## 10.6 Protein Tools

Maestro has tools for a number of operations on proteins: aligning and splicing protein structures, assigning secondary structures, reporting on protein properties, generating Ramachandran plots, and generating interaction energies for rotamers and ligand torsions in a complex.





**Figure 10.8.** The Source Structures panel.

### 10.6.1 Assigning Protein Secondary Structure

The Assign Secondary Structure command on the Tools menu provides a way of assigning secondary structure labels to a protein. The assignment occurs in two stages. First, all inter-backbone hydrogen bonds are identified. Second, a search is made for hydrogen-bonding patterns representing helices and strands. The assignment is used for the display of ribbons, the use of some color schemes, and for the Workspace sequence viewer.

### 10.6.2 Viewing Reports on Protein Properties

Reports on various properties of the protein that is in the Workspace are presented in the Protein Reports panel, which you open by choosing Tools → Protein Reports. The Display option menu lists the various protein properties for which reports can be generated. When you choose an item from the menu, the table is updated with the relevant report.

The table displays the label for each residue or residue pair in the report in the first column, and the report data in the remaining columns. Clicking a row marks the residue or the relevant part of the residue in the Workspace, and zooms in on the residue. Clicking a column heading

sorts the table by the data in the column. Repeated clicking cycles through ascending order, descending order, and original order.

*Table 10.1. Display menu items in the Protein Reports panel*

<b>Item</b>	<b>Description</b>
Steric Clashes	Ratio of the interatomic distances to the sum of the atomic (van der Waals) radii from the force field. The threshold is 0.85.
Bond Length Deviations	Deviation from the ideal value derived from Engh and Huber. The RMSD is reported at the bottom.
Bond Angle Deviations	Deviation from the ideal value derived from Engh and Huber. The RMSD is reported at the bottom.
Backbone Dihedrals	G-factors for backbone dihedrals (see below for definition), along with dihedral angles. Less negative (closer to zero) means that the combination of angles is more probable.
Sidechain Dihedrals	G-factors for side-chain dihedrals (see below for definition), along with dihedral angles. Less negative (closer to zero) means that the combination of angles is more probable.
G-Factor Summary	G-factors for backbone dihedrals, side-chain dihedrals, and the sum of the two.
Average B-Factors	Average B-factors (temperature factors) for the backbone and the side chain for each residue, and their standard deviations.
Gamma-Atom B-Factor	B-factor for the gamma atom in each residue.
Peptide Planarity	RMSD of the atoms in the peptide linkage from the plane that minimizes the RMSD.
Sidechain Planarity	For side chains that have nominally planar groups, RMSD of the atoms in the planar groups from the plane that minimizes the RMSD.
Improper Torsions	For side chain atoms that are nominally planar, RMSD of the improper torsion for these atoms.
C-alpha Stereochemistry	Stereochemistry of the C-alpha atoms.
Missing Atoms	Residues for which atoms are missing from the structure.

G-factors are calculated by binning the dihedral angles from a collection of high-resolution structures into 10-degree ranges, and calculating the probability of a pair of angles lying in a given range. The G-factor is the logarithm of this probability. If there are no values in a given range, the G-factor is reported as “disallowed”.

Residue	Backbone	BBSStdDev	Sidechain	SCStdDev
A: GLU 4	54.536	1.754	67.461	25.057
A: ARG 5	45.048	3.748	48.167	21.447
A: PRO 6	31.414	30.769	37.38	5.348
A: THR 7	27.8	1.45	29.586	0.146
A: PHE 8	27.454	21.238	25.934	4.135
A: TYR 9	27.845	2.962	22.827	1.221
A: ARG 10	27.058	4.281	44.764	27.686

Structure average: 27.801

Update

**Figure 10.9. The Protein Reports panel.**

### 10.6.3 Protein Reliability Reports

The Protein Reliability Report panel displays a simple graphical representation of various metrics that indicate the reliability or quality of a protein structure, and in particular, X-ray structures of proteins. To open the panel, choose Tools → Protein Reliability Report.

To analyze a protein for reliability, you must first display it in the Workspace. If a report has already been generated for a protein, and it is displayed in the Workspace, the report is displayed immediately.

Next, choose which part of the protein to analyze, from the Analyze option menu:

- Entire structure—Analyze the entire structure that is in the Workspace.
- Region around ligand—Analyze the region that includes the ligand and all residues that have atoms within a specified distance of the ligand.

When you choose this option, a text box, a Pick ligand option, and a Shell text box are displayed to the left of the menu. To identify the ligand, select the Pick ligand option and pick a ligand atom in the Workspace. The identity of the ligand is displayed in the text box. To set the distance, use the Shell text box. The default distance is 10 Å.

- Custom region—Analyze the region that includes a custom selection of residues.

When you choose this option, a text box and a Select button are displayed to the left of the menu. To select the residues for the region, click Select and use the tools in the Atom Selection dialog box. The ASL expression for these residues is displayed in the text box.

If you want to include X-ray diffraction data in the analysis, select **Use diffraction data** and click **Browse**. A file selector opens, in which you can locate and select the file that contains the diffraction data. The file name is displayed in the text box. You can also type the full file name into the text box. The X-ray data are used to calculate real-space R-factors and correlation coefficients.

When you have finished defining the input and the analysis region, click **Run** to generate the report. After the job finishes, the results are displayed in the display area.

This area displays a visual representation of the metrics for protein reliability. For each metric a circle is drawn that represents the quality of that metric. It is colored red if the deviation from acceptable values is larger than a threshold, and green if the deviation is smaller. The radius of the circle indicates the magnitude of the metric. Circles are still drawn for metrics that were not calculated, but they are not colored. For large deviations, the circles can overlap other circles.

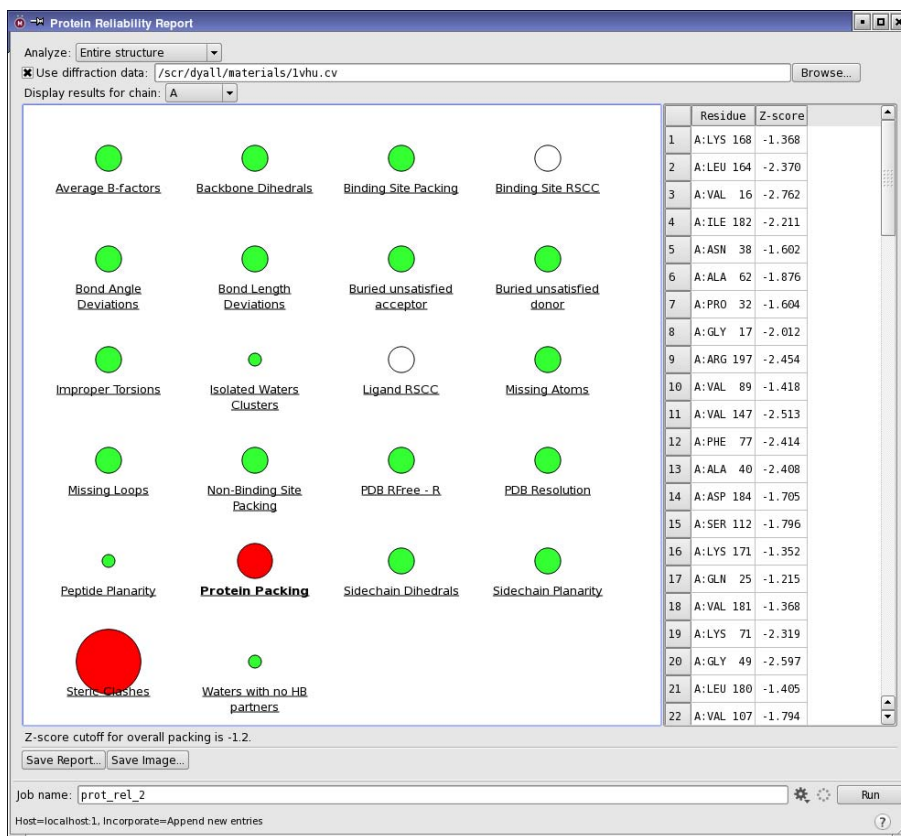


Figure 10.10. The Protein Reliability Report panel.

The intention of the display is to provide a quick means of determining if the protein structure is reliable, and which aspects of the structure deviate from acceptable values.

The metrics that are used to assess the quality of the protein structure are described in [Table 10.2](#), with the threshold values for marking a problem. Some metrics require X-ray reflection data for their evaluation. Some apply to the entire protein, others apply to the region that is analyzed.

*Table 10.2. Protein reliability metrics.*

<b>Metric</b>	<b>Description</b>	<b>Cutoff</b>
Average B-factors	Number of residues in the analyzed region whose average B-factor is larger than 100.	100
Backbone dihedrals	Number of abnormal backbone dihedrals in the analyzed region (those in the disallowed region of a Ramachandran plot).	1
Binding site packing	Number of residues in sequences of three or more consecutive residues in the binding site that have Z-scores less than • 4.0.	0
Binding site RSCC	Real-space correlation coefficient for the binding site. Can help to identify cases where the binding site is poorly built.	0.9
Bond angle deviations	Number of bond angles in the analyzed region that deviate by more than 4 standard deviations from standard bond angles.	1
Bond length deviations	Number of bond lengths in the analyzed region that deviate by more than 4 standard deviations from standard bond lengths.	1
Buried unsatisfied acceptor	Number of buried H-bond acceptors in the analyzed region that do not have hydrogen bonds. Most acceptors buried in a protein are part of a hydrogen-bonding network.	1
Buried unsatisfied donor	Number of buried H-bond donors in the analyzed region that do not have hydrogen bonds. Most donors buried in a protein are part of a hydrogen-bonding network	1
Improper torsions	Number of improper torsions in the analyzed region that exceed 10°.	0
Isolated water clusters	Number of water clusters that are not hydrogen-bonded to anything else.	0
Ligand RSCC	Real-space correlation coefficient for the ligand. Can help to identify cases where the ligand is poorly built or the density does not support ligand placement.	0.9
Missing atoms	Number of atoms missing from the analyzed region.	0
Missing loops	Number of loops missing from the entire structure.	0
Non-binding-site packing	Number of residues that are not in the binding site in which the Z-scores are less than • 4.0 in sequences of three or more residues.	0

Table 10.2. Protein reliability metrics. (Continued)

Metric	Description	Cutoff
PDB resolution	X-ray structure resolution.	2.5 Å
Peptide planarity	Number of peptide dihedrals that are greater than 20°.	0
Protein packing	Average packing environment of the protein, measured by the average Z-score of all residues in the protein. A problem is flagged if the Z-score is more negative than the threshold. High-quality structures have a uniform distribution of atoms in the core of the protein.  The presence of holes in the core can be an indicator of poorly built side chains or backbone, or incorrect threading of the sequence through the density.	• 1.2
Side-chain dihedrals	Number of dihedral angles in the side chains that are in the disallowed region of a Ramachandran plot.	0
Side-chain planarity	Number of side chains that are expected to be planar whose RMSD to the ideal plane exceeds 0.5Å.	0
Steric clashes	Number of abnormally short interatomic distances.	1
Waters with no HB partners	Number of waters that do not form hydrogen bonds at all.	0

The results of the analysis can be displayed for each chain separately, or for the entire protein. Use the Display results for chain option menu to select the chain or the entire protein (All).

If you click on the title of a metric, the values for that metric are displayed in a table, to the right. For metrics whose values lie outside acceptable ranges, the unacceptable values are displayed in the table. The section is blank initially, and is cleared if you choose a metric whose values are all acceptable.

Below the display area an informational message on metrics whose values lie outside the acceptable range is shown, when you click on the metric in the display area. It specifies the cutoff for acceptable values, and suggests possible reasons that the values might lie outside the range.

You can save a copy of the report in a text file (.txt), by clicking Save Report. The report lists metrics and their values. You can also save an image of the display area to a file, in PNG, JPEG, or TIFF format. The Save Image button opens a file selector, in which you can choose the image format and save the file.

## 10.6.4 Ramachandran Plots

The Ramachandran Plot panel displays a plot of the dihedral angles  $\phi$  and  $\psi$  for each residue in the protein that is displayed in the Workspace. To open the panel, choose Tools → Ramachandran Plot. This panel is useful for identifying residues that fall in disallowed regions of protein dihedrals, so that adjustments can be made to the protein geometry. After adjusting the geometry, click Refresh to redisplay the plot. You can only display a plot for one entry at a time.

The plot area displays a plot of protein dihedrals for all residues in the protein. The plot is organized as follows:

- Glycine is plotted as triangles, proline is plotted as squares, all other residues are plotted as circles.

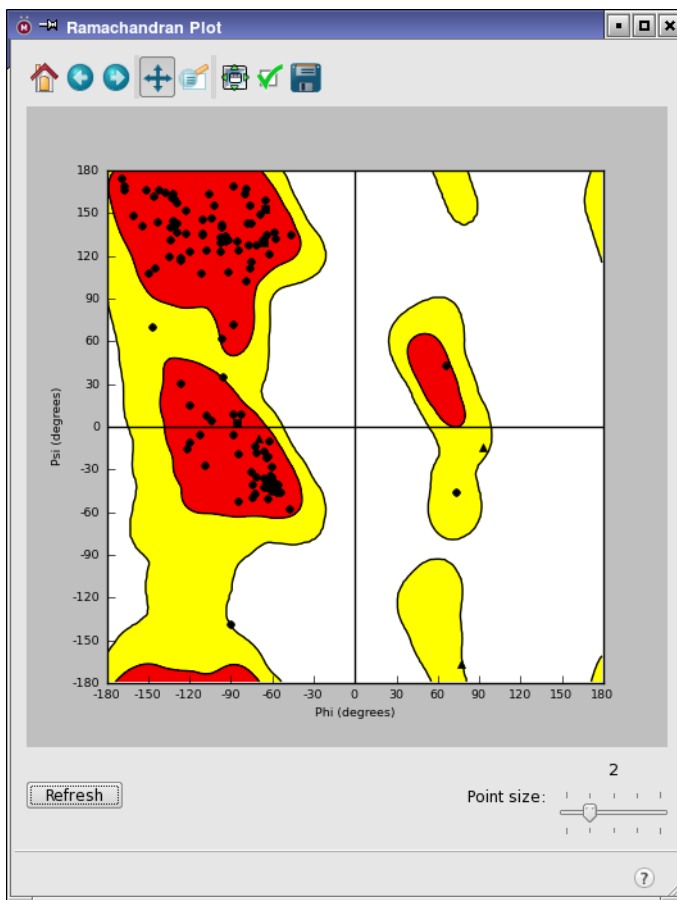


Figure 10.11. The Ramachandran Plot panel.

- The orange regions are the “favored” regions, the yellow regions are the “allowed” regions, and the white regions are the “disallowed” regions.

The following actions can be performed on the plot:

- Clicking on a point zooms the Workspace image in to that residue. The point is displayed as an outline instead of solid black. The residue information is displayed at the top of the panel and the residue is highlighted in the Workspace and the sequence viewer.
- Pausing the pointer over a point displays information for that residue at the top of the panel, and highlights the residue in the Workspace and the sequence viewer. When you move the pointer off the point, the display returns to that of the selected point, if there is one.

The size of the points on the plot can be adjusted using the Point size slider.

The panel has a toolbar that you can use to configure the plot or to save an image of the plot. The toolbar buttons are described below.



**Reset**

Reset the plot to the original pan and zoom settings.



**Back**

Display the previous view of the plot in the view history



**Next**

Display the next view of the plot in the view history



**Pan/zoom**

Pan the plot by dragging with the left mouse button, zoom by dragging with the right mouse button.



**Zoom to rectangle**

Drag out a rectangle on the plot to zoom in to that rectangle.



**Configure subplots**

Configure the margins and spacing of each plot in the panel.



**Edit axis and curve parameters**

Make settings for the title, range, labeling, and scale of the axes; the color, style, and width of lines; and the color, style, and size of markers.



**Save image**

Save an image of the plot to file. Opens a file selector in which you can browse to a location, select the image format, and name the image.



**Copy to clipboard**

Copy an image of the plot to the clipboard. You can then paste it into another application. This button is only available in some panels.



## 10.6.5 Energy Profiles of Torsional and Rotamer States

The Rapid Torsion Scan panel enables you to scan the orientations around a ligand bond or rotamer states of a selected protein residue and see a breakdown of the energy for each orientation or state.

To open the Rapid Torsion Scan panel, choose Tools → Rapid Torsion Scan.

The panel has two options for selecting the torsional states to sample:

- **Pick ligand bond to rotate**—Select this option and pick a bond in the Workspace to define the bond to rotate around. You should pick the bond nearer to the end of the bond that is rotated. The bond is scanned by default at 30° intervals, but you can adjust the interval with the Angle increment slider, which sets the angle interval to integer divisors of 360° from 1° to 30°. The number of states generated is reported in the Number of rotamers text box. If you subsequently change the angle increment, click **Recalculate** to regenerate the rotamer states.
- **Pick standard protein residue to sample**—Select this option and pick a protein residue for which you want to see energetic information on the rotamer states.

When you pick the ligand bond or the residue, a calculation with the OPLS\_2005 force field is performed to evaluate the interaction energy for each rotamer or torsional angle, and the results are presented in the Rotamer states table. As well as the total energy, the contributions from the electrostatic component and van der Waals plus internal components are presented.

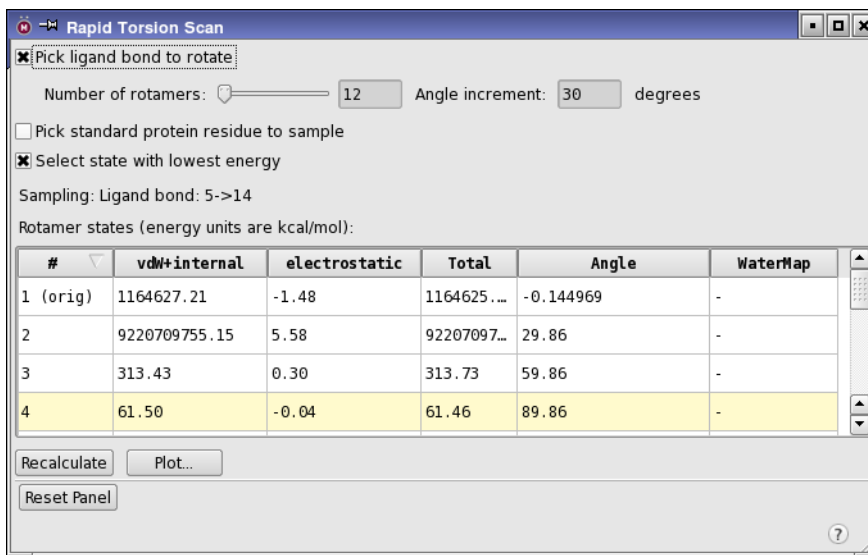


Figure 10.12. The Rapid Torsion Scan panel.

Rotamer states are identified by their probability, and the bond or residue is identified above the table. The original rotamer state does not have an associated probability, because the probability is derived from a data set of rotamer states and this state might not be in the data set. The table can be sorted by clicking in a column header.

If you select **Select state with lowest energy**, the lowest energy state is selected in the table and displayed in the Workspace. Selecting a row in the table also displays the state in the Workspace. The structure in the Workspace is changed, and so the corresponding project entry will also be changed. The original state is the first state in the table, which you can select to return to the initial state.

To see a plot of the rotamer states as a function of the angle (for ligands) or rotamer state number (for protein residues), click **Plot**, which opens the **1D Plot** panel with a display of the plot. For more information on this panel, see [Section 11.2 on page 290](#).

### 10.6.6 Ligand Interaction Diagrams

The **Ligand Interaction Diagram** panel allows you to generate and display a 2D diagram of the interactions between a ligand and various protein residues.

To open the **Ligand Interaction Diagram** panel, choose **Tools** → **Ligand Interaction Diagram**, or click the **Lig. Int.** button on the **Project** toolbar.



The diagram is generated automatically from the structures in the Workspace. If you have more than one ligand in the Workspace, the first is used, and you can choose any of the other ligands from the **Ligand** option menu.

The orientation of the ligand can be chosen to match the Workspace orientation, or to give the best 2D representation. To match the Workspace orientation, select **Sync with 3D**. When you rotate the structure in the Workspace, the diagram is redrawn to match the Workspace orientation. To give the best 2D orientation, click the **Best 2D View** button on the toolbar.



You can also change the orientation by using the toolbar buttons. These perform the same functions as those on the **2D Sketcher** toolbar—see [Section 5.5.2 on page 90](#) for details.

The set of residues that appear in the diagram is determined by the cutoff specified in the **Cutoff** text box. All residues that have any atom within the specified distance of any ligand atom are included in the diagram. If you change this value, the diagram is regenerated with the new set.

In the diagram, residues are represented as colored spheres, labeled with the residue name and residue number. The colors indicate the residue (or species) type:

- red—acidic (Asp, Glu)
- green—hydrophobic (Ala, Val, Ile, Leu, Tyr, Phe, Trp, Met, Cys, Pro)
- purple—basic (His, Lys, Arg)
- blue—polar (Ser, Thr, Gln, Asn, His, Hie, Hid)
- light gray—other (Gly, water)
- darker gray—metal atoms

Interactions with the protein are marked with lines between ligand atoms and protein residues:

- Solid pink—H-bonds to the protein backbone
- Dotted pink—H-bonds to protein side chains
- Green—pi-pi stacking interactions
- Orange—pi-cation interactions

Ligand atoms that are exposed to solvent are marked with gray spheres. The protein “pocket” is displayed with a line around the ligand, colored with the color of the nearest protein residue. The gap in the line shows the opening of the pocket.

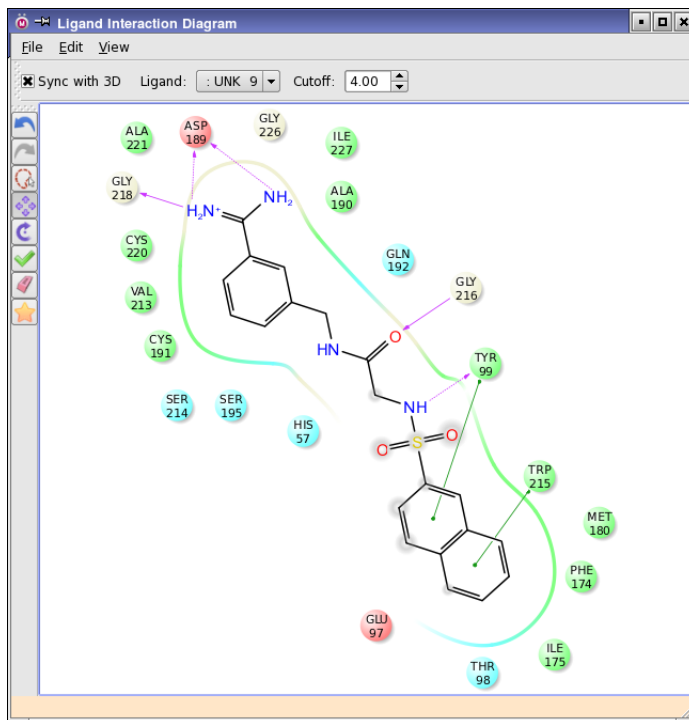


Figure 10.13. The Ligand Interaction Diagram panel.

The details of the representation can be displayed in the panel, by choosing View → LID Legend. Likewise, the title of the ligand entry can be displayed by choosing View → Scene Title. You can control aspects of the formatting, such as the sphere radii, the font size, the line widths, residue by choosing Edit → Preferences, and making settings in the panel that opens.

If you want to save the diagram in an image file, choose File → Save Screenshot, or press CTRL+ALT+P (⌘⌘P). A file selector opens, so you can browse to a location and name the file. The image can be saved in PNG or EPS format, and you can specify the size of the image in pixels or the size and resolution of the document in inches and pixels/inch (dpi).

You can also generate diagrams from the command line as an image file—see [Section 4.4](#) of the *General Utilities* manual.

### 10.6.7 Protein Splicing

The Protein Splicing tool can be used to take a segment of one protein (the source) and replace a segment of another protein with the source segment. The proteins are aligned temporarily if they are not already aligned, so that the segment can be simply transferred between the source and the destination. The regions around the attachment points are minimized, but otherwise no change is made to the spliced segment. This is intended to be a quick means of transferring residues from one protein to another.

Prior to splicing a segment of a protein into another protein, you may want to perform a structural alignment of the two proteins, so that the termini of the desired source and destination segments are aligned to each other. This gives you more control over the alignment than the automatic global alignment done as part of the procedure.

Once the source segment is defined, possible attachment points on the (aligned) destination protein are identified. The attachment atoms are the carbonyl carbon on the C-terminus end

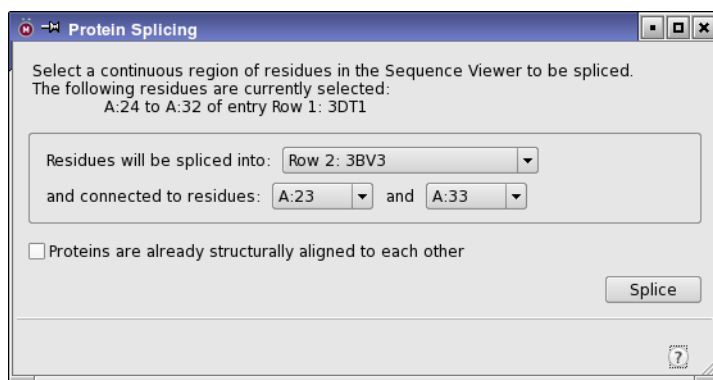


Figure 10.14. The Protein Splicing panel.

and the nitrogen on the N-terminus end. Any attachment atoms in the destination that are within 8 Å of the attachment atoms of the source segment are considered as potential attachment points. Of these, the default is selected to preserve the residue numbering if possible, otherwise the attachment atom that forms the shortest peptide bond with the segment is taken. The preservation of the numbering assumes that the splicing is being done between two different structures of the same (or similar) protein, with the same residue numbering.

The splicing is done by temporarily aligning the source protein to the destination if necessary; extracting the source segment and deleting the destination segment (between the attachment points); assigning the destination chain ID to the spliced segment and renumbering the residues to continue from the N-terminal attachment residue numbering. If a duplicate residue number is found, the residue in the spliced segment is assigned a number that is higher than any found in the destination chain. The new segment is attached at the attachment points (or point, for a terminal attachment), and all atoms within 6 bonds of the attachment points are minimized. A new project entry is created for the modified protein.

Apart from the minimization around the attachment points, no attempt is made to relieve strain or clashes with the rest of the target protein. Once the splicing is done, you should run a refinement on the spliced segment and its local environment.

#### **To splice a segment of one protein (the source) into another protein (the destination):**

1. Include both proteins in the Workspace.

You can include more than one protein in the Workspace, but only one protein can be selected as the destination. You might want to do this to identify variable and conserved regions in a set of related proteins, to guide the selection of the segment to splice.

2. If the proteins are already aligned, select Proteins are already structurally aligned to each other.

This should be done before defining the source segment: once it is defined, the proteins are aligned temporarily if they aren't already.

3. Select a contiguous set of residues in the source protein.

It is probably easiest to do this in the sequence viewer, which is displayed automatically when you open the panel. If you make the selection in the Workspace, it is filled out to entire residues. You must make sure the residues are attached in a continuous chain.

Once the residues are selected, the segment selected is reported in the top part of the panel, and the option menus are filled in with the list of possible destination proteins and the residues on the destination to which the splicing could be done.

4. Choose the destination protein, if you have more than two proteins in the Workspace.

5. Change the selection of the attachment residues, if necessary.

If you need to identify the residues, you should be careful not to select a residue in the Workspace, as this will change the source segment. You can identify the residues by using atom feedback: pause the pointer over an atom in the Workspace, and its identity, including the residue number, is displayed in the status bar.

If you want to splice the tail of a protein onto another protein, you can choose **None** as an attachment residue on the C- or the N-terminal end. You should only do this for one attachment point: setting both to **None** results in an error message.

6. Click **Splice**.

The segment is spliced into the destination protein, and the new protein is added to the project as a new entry and replaces the Workspace. The panel then closes.

## 10.6.8 The Multiple Sequence Viewer

The Multiple Sequence Viewer panel is an alignment, visualization, and manipulation toolkit for multiple sequences. It is described in a separate document, *Multiple Sequence Viewer*.

To open the Multiple Sequence Viewer panel, choose **Tools** → **Multiple Sequence Viewer**.

## 10.7 Assigning Bond Orders and Partial Charges

The **Assign Bond Orders** command on the **Tools** menu assigns bond orders to structures that do not have the correct bond orders, as follows:

- If you have a Workspace selection that is 300 atoms or less, bond orders are assigned for all the selected atoms.
- If the selection has more than 300 atoms, bond orders are assigned for all residues in the selection that do not have multiple bonds.
- If there is no selection, bond orders are assigned for all residues in the Workspace that do not have multiple bonds.

The assignment is based on a range of factors, including connectivity, bond length, bond angles and dihedral angles. Occasionally the bond order cannot be assigned, or is assigned incorrectly. You should always check your structure after using this command, especially for bonds that are unusual in any way. If you find any errors, you can correct them with the **Build** toolbar buttons—see [Section 5.7 on page 96](#).

If you have built a structure using **Draw** mode in the **Build** panel, you should change the bond orders manually, because the structure is unlikely to meet the criteria for bond lengths, angles and dihedrals required for successful bond order assignment.

Assignment of bond orders is a necessary preliminary to hydrogen addition. If the bond orders are incorrect, hydrogen addition will place too many or too few hydrogen atoms.

The **Assign Partial Charges** command on the Tools menu assigns partial charges to the structures in the Workspace, based on the OPLS\_2005 force field. These partial charges can be used for many purposes, such as coloring a surface by partial charge and displaying the dipole moment of the molecule. If the structure does not have explicit hydrogens, the partial charges for the implicit hydrogens are added to the partial charge for the heavy atom to which they are implicitly attached.

## 10.8 Ligand Filtering

If you want to filter a set of ligands based on their properties, you can do so in the Ligand Filtering panel. This panel allows you to set up filtering criteria for a set of structures, which are represented as a set of conditions on Maestro properties, certain predefined feature counts, or counts of SMARTS patterns for functional groups. When you have set up the criteria, you can run a job to apply the criteria to the structures and return those that match or that do not match.

To open the Ligand Filtering panel, choose Ligand Filtering from the Tools menu. A brief description of the procedure is given here, with details in the subsections below.

### To filter a set of structures by various structural attributes:

1. Select a structure source from the **Use structures from** option menu. If you choose a file, specify the file name or browse to locate it.
2. Choose how matching is defined under **Ligand matches if**.
3. Choose what to do with the ligands that match, using the **Matching ligands** options.
4. If you want to mark the ligands that match in the output, select **Set boolean property** and provide a property name.
5. Select a property, general attribute, or functional group from the lists in one of the tabs, and construct a criterion using the text boxes and option menus.  
  
You can define upper and lower limits on a property value by using both text boxes and option menus and a boolean operator to connect the two limits.
6. Click **Add** to add the criterion to the **Filtering definitions and criteria** list.
7. Repeat the last two steps to add as many criteria as you like.
8. Click **Start** to set up and start the job.

The job runs the `ligfilter` utility, described in [Section 2.4](#) of the *General Utilities* manual.

If you want to start again or create a new filter, click **Reset**, to clear the entire panel. If you want to write the criteria file without running a job, click **Write**. In the dialog box that opens, enter a name for the file, which is written to the current directory with the extension `.lff`.

### 10.8.1 Selecting a Structure Source

The **Use structures from** option menu allows you to choose from three structure sources:

- **Workspace**—Filter the structures that are included in the Workspace. These structures are written to an input file, by entry.
- **Project Table**—Filter the structures that are selected in the Project Table. These structures are written to an input file, by entry.

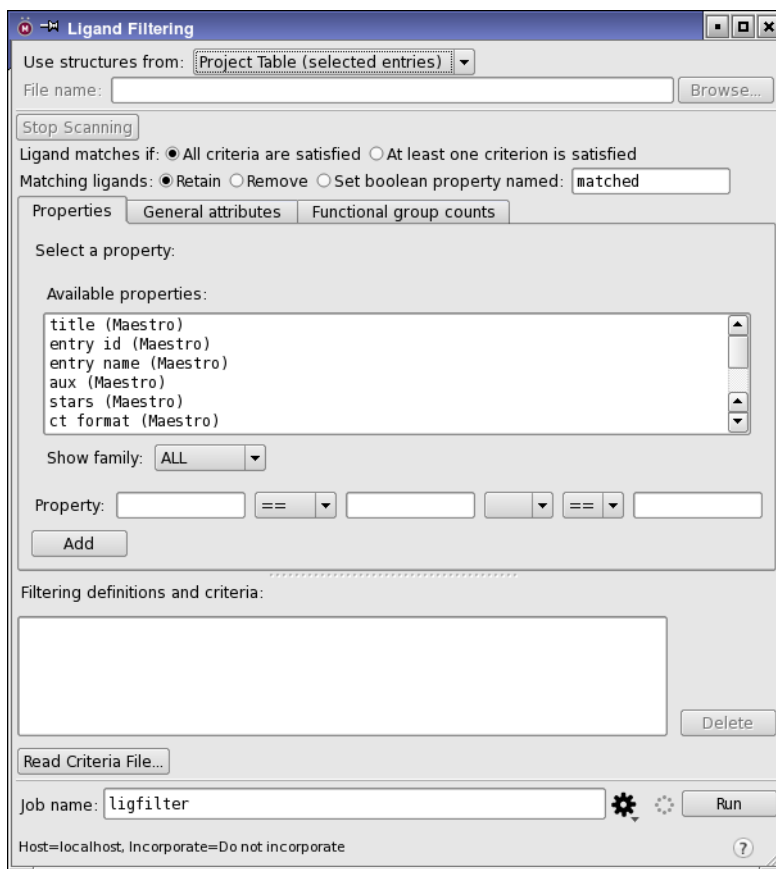


Figure 10.15. The Ligand Filtering panel.



- **File**—Filter the structures in the file specified in the Input file text box. You can click Browse to navigate to the desired file. When you have selected or entered a file, the file is scanned for properties to list in the Properties tab. If you want to stop this scan, click Stop scanning.

## 10.8.2 Defining the Matching Method

There are several choices for how the matching is done. First, you can choose whether the ligand must meet all criteria or only one criterion. This choice is made with the Ligand matches if options:

- **All criteria are satisfied**—The ligand must match all criteria. This choice corresponds to connecting each criterion by a logical AND operator.
- **At least one criterion is satisfied**—The ligand must match one of the criteria. This choice corresponds to connecting each criterion by a logical OR operator.

Once you have decided how to match the criteria, you must decide next whether to keep the ligands that match, discard them, or mark them. This you can do with the Matching ligands options:

- **Retain**—Write the ligands that match to the output structure file. Ligands that do not match are not written out.
- **Remove**—Write the ligands that do not match to the output structure file. Ligands that match are not written out.
- **Set boolean property**—Write all ligands to the output structure file, and for each ligand, set a Boolean property that indicates whether it matched or not.

You can name the Boolean property in the Property name text box. This name is the name that is displayed in the Project Table. By default the name is `matched`, and can be filtered with the `ligfilter` family of properties. The property name cannot contain spaces. When the visible name is displayed, any underscores are replaced with spaces for display purposes.

## 10.8.3 Defining Matching Criteria

The center section of the panel has three tabs, for setting up criteria using different classes of structural attributes. Each tab has the following common features:

**List of structural attributes**—This list contains the available structural attributes (properties, general attributes, or functional groups). You can select a single item from this list. The selected item is displayed in the first text box below the list, which is labeled with the structural attribute class. In the Properties tab, there is a Show family option menu below the list. You can use this menu to limit what is shown in the list to a single property family (e.g. QikProp).

**Criterion specification text boxes and option menus**—Below the list is a set of text boxes and option menus that you use to construct a criterion. The first text box lists the structural attribute selected from the list. To define a condition on the structural attribute, choose a relational operator from the leftmost option menu and enter a value in the text box immediately to the right of it. If you want to define two conditions, choose a Boolean operator (AND or OR) from the next option menu, then choose a relational operator from the option menu and enter a value in the text box that are to the right of the Boolean operator.

**Add button**—This button adds the criterion to the filter. The criterion is displayed in the Filtering definitions and criteria text area.

Below the tabs is the Filtering definitions and criteria text area, which lists the criteria from all tabs that make up the filter, one per line. Property criteria are given in terms of their internal names in this list, rather than the external names as they are in the Select a property list. If you want to delete one or more criteria, select them in this text area and click Delete.

You can read an existing file of criteria by clicking Read criteria file, and navigating to the file in the file selector that is displayed. The file has the extension `.lff`. The contents of this file replaces the contents of the Filtering definitions and criteria. Once the criteria are loaded, you can add to them, or delete them.

## 10.8.4 Defining New Matching Patterns

In the Functional Group Counts tab, you can define new functional groups that can be used to match the ligands. The functional groups are defined by SMARTS patterns. Here we use a broad definition of a functional group that encompasses any set of atoms that is defined by some atom type and connectivity pattern.

You can set up a new functional group in the Add Definition dialog box, which you open by clicking New.

Each pattern that is added to the definition can either be “included” in the definition or “excluded” from the definition. For a chemical feature to match the definition, it must match all of the included patterns, and it must not match any of the excluded patterns. So, for example, if you wanted to match all oxygen atoms that were not in alcohols, you could include O, and exclude Alcohols.

To add an existing pattern to the definition, select the pattern in the list and click Include or Exclude. The pattern name is displayed in the SMARTS expression or pattern name text box when you select it. If you want to view the definition of an existing pattern, click View. The SMARTS string for the pattern is displayed in a dialog box.

To add a SMARTS pattern, enter the SMARTS expression in the text box above the list, and click Include or Exclude. You can also select atoms in the Workspace, then click Get From Selection to add a SMARTS pattern for the selected atoms to the text box.

When you click Include, the pattern is added to the list in the lower part of the panel, preceded by a + sign. Likewise, when you click Exclude, the pattern is added to the list in the lower part of the panel, preceded by a – sign. You can delete patterns from this list by selecting them and clicking Delete, and you can clear the list by clicking Delete All.

Before you click Add to add the new definition, ensure that you have named it in the Name of new functional group text box.

### 10.8.5 Eliminating Duplicate Ligands

Another task that is related to filtering is the elimination of duplicate ligands. This task can be done in the Merge Duplicates panel, which you open with Tools → Merge Duplicates. The elimination is done by comparing SMILES strings, and the output is either a SMILES file or a

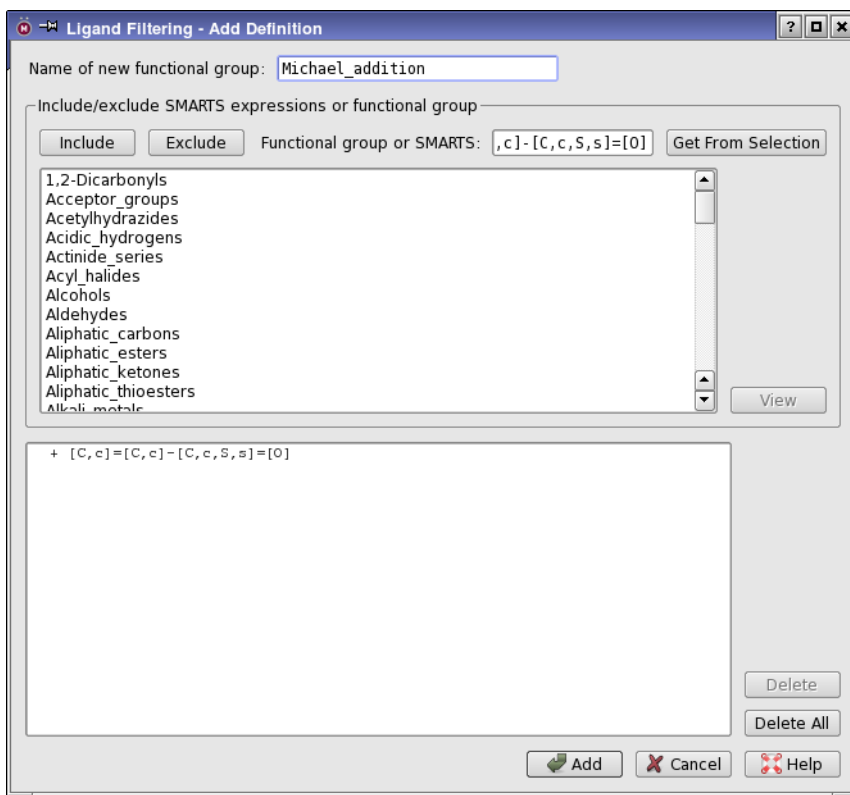


Figure 10.16. The Add Definition dialog box.

2D SD file; in either case the output contains no 3D information other than chirality properties. This tool is therefore most useful when you plan to prepare the structures for modeling with LigPrep, either directly or as part of another workflow. You can neutralize and desalt the structures in the process of merging, and you can merge property values into a string, where a given property has a value for more than one of the duplicates.

## 10.9 Minimizing Structures

For a quick minimization of a structure or part of a structure, the Tools menu offers a few choices. The Minimize option menu provides for minimization of the selected atoms, all atoms, or the ligand. The Structure Sculpting tool enters a mode in which you can move individual atoms and the environment of the atom is minimized after the move. These tools are described in more detail in [Section 5.9.5](#) and [Section 5.9.6 on page 107](#).

## 10.10 Visualization Tools

Maestro includes a range of visualization tools for various kinds of data—in addition, of course, to the display of structures in the Workspace. These tools are listed below, with references to the location of their descriptions. Descriptions are also given in the help.

- **Plotting.** The plotting tools enable you to plot data associated with project entries. These tools are described in [Chapter 11](#).
- **Surfaces.** Maestro can generate surfaces and display surfaces generated by various computational programs. Generation and display of surfaces is described in [Chapter 12](#).
- **Vibrational animation.** Vibrational frequencies generated by Jaguar can be animated in the Workspace, via the Project Table. The animation tool is described in [Section 3.9.4](#) of the *Jaguar User Manual*.
- **Ramachandran plots.** The tool for generating and displaying Ramachandran plots of protein dihedrals is described in [Section 10.6.4 on page 267](#).
- **Ligand Interaction Diagram.** This tool displays a simplified representation of protein-ligand interaction, and is described in [Section 10.6.6 on page 270](#).
- **Coordinate Scan Plots.** These panels display plots of energy as a function of one or two coordinates, and are described in [Section 11.2 on page 290](#). MacroModel and Jaguar can generate information for plotting in these panels.
- **Force Field Viewer.** This tool displays the interactions generated from the various force-field terms in a MacroModel calculation, and is described in [Section 5.4](#) of the *MacroModel User Manual*.

- **Trajectories.** The Trajectory panel allows you to display trajectories (animated) from MD simulations that were generated by Desmond or Impact. The viewer is described in [Section 5.1](#) of the *Desmond User Manual*.



# Plotting

Maestro's Plot facility allows you to generate scatter plots from data in the Project Table. Each plot can consist of multiple data sets, and each data set can represent up to four properties, by use of location, color, and plot symbol size to represent the property values. The plots interact with the Project Table selection and inclusion, so that you can use the plot to select entries and include them in the Workspace. Plots are stored in the project.

For coordinate scans in one or two coordinates, such as generated by MacroModel or Jaguar, Maestro provides special plotting capabilities, in the Plot of One-Coordinate Scan panel and Plot of Two-Coordinate Scan panel.

## 11.1 Scatter Plots

Scatter plots are generated from data in the Project Table for the selected entries. The plots are managed in the Manage Plots panel. From this interface you can add, edit, view and delete plots. Scatter plots can also be generated from applications such as Strike and Phase, to display predictions against the experimental data.

### 11.1.1 Managing Plots

The Manage Plots panel is used to add, edit, view, and delete plots. To open the Manage Plots panel, choose **Table → Plot**, or click the **Plot** button on the toolbar.



This panel lists the plots that are stored in the project. You can select multiple plots in this list, and apply the following actions to them:

- **Delete**—delete the selected plots.
- **Show**—display the plot panels for the selected plots. Double-clicking a single plot shows that plot.
- **Hide**—close the plot panels for the selected plots

To rename a plot, select it in the list, click **Rename**, then enter the new name in the dialog box that opens and click **OK**. This is the name that appears in the title bar of the Scatter Plot panel. You can use spaces in the name.

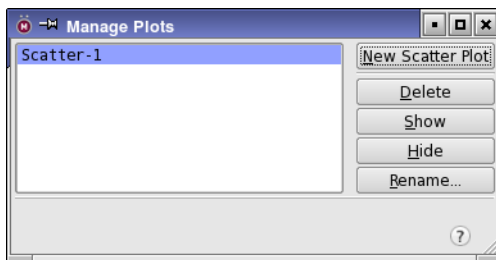


Figure 11.1. The Manage Plots panel.

### 11.1.2 Creating Plots

Plots are created from property data in the Project Table. To plot data, you must therefore have at least one entry in the Project Table. The following instructions create a simple scatter plot of two properties.

#### To create a simple scatter plot:

1. Select the entries in the Project Table whose data you want to plot.
2. Choose Table → Plot or click the Plot button on the toolbar.



The Manage Plots panel opens.

3. Click New Scatter Plot.

A new scatter plot panel opens, with a blank plotting area.

4. Choose the property for the  $x$  axis and the  $y$  axis.

You can make the choice from the option menus, or click Select to open a property selector, in which you can restrict the list of properties by family or by filtering.

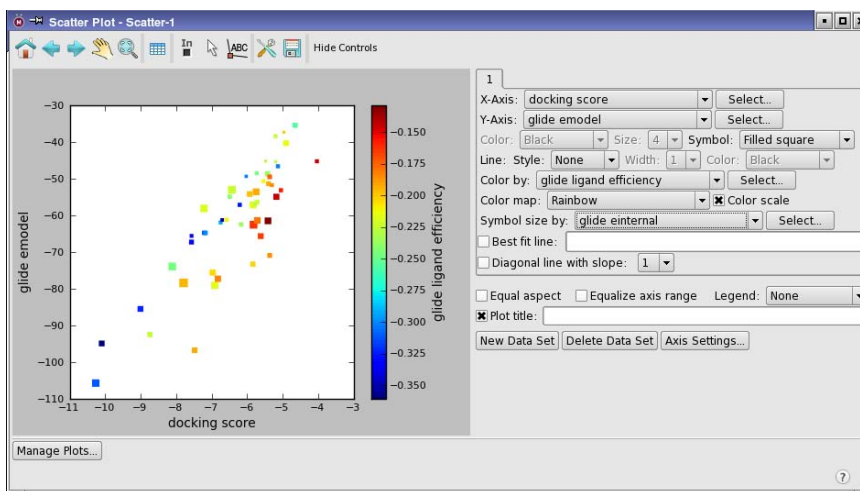
When you have chosen properties for both axes, data points appear in the plotting area.

From here you can continue on to make further plot settings. These settings are described in [Section 11.1.3 on page 285](#).

There are several other possibilities offered for creating more complex plots:

- You can represent a third property by coloring the plot symbols with a color map. To do so, choose the property from the Color by option menu (or click Select), then choose a map from the Color map option menu.





**Figure 11.2. A Scatter Plot panel with four properties represented.**

- You can represent a fourth property by the size of the plot symbols. To do so, choose the property from the Symbol size by option menu (or click Select).
- You can add data sets to the plot by clicking New Data Set. When you do so, a new tab is displayed with the same controls as the first tab. You can then select the properties you want to display in the same way as you did for the first data set. To delete data sets, display the tab for the data set you want to delete, and click Delete Data Set.

### 11.1.3 Changing Plot Settings

The settings that govern the appearance of the plot itself can be made in the tab for the data set. Settings for the axes and the color bar can be made in the Axis Settings dialog box.

Each data set has its attribute settings in a tab on the right of the panel. These settings fall into several classes: the properties that are represented, the plot symbols and line style used, and the display of additional lines that are related to the data. These controls can be hidden by clicking Hide Controls on the toolbar, and redisplayed by clicking Show Controls.

#### 11.1.3.1 Changing the Plotted Properties

The properties that are plotted on the two axes can be changed from the X-Axis and Y-Axis option menus, or by clicking the corresponding Select button and choosing the property in the property selector that is displayed. The property selector allows you to show properties from a given property family and to filter the properties by matching a text string that can include wildcard characters.

Two more properties can be represented on the plot, by using the color of the plot symbols and their size. To change the property that is represented by color, choose the property from the Color by option menu (or click Select to use a property selector), then choose a map from the Color map option menu. To change the property that is represented by symbol size, choose the property from the Symbol size by option menu (or click Select).

### 11.1.3.2 Changing the Plot Symbols and Lines

The color of the plot symbols, their point size, and the shape of the symbol can be changed by choosing from the Color, Size, and Symbol option menus. If you choose a property to color the symbols by, the Color option menu is not available. Likewise, if you choose a property to map to the symbol size, the Size option menu is not available.

The line style, width, and color can be changed by choosing from the Style, Width, and Color option menus to the right of the Line label. If you do not want a line connecting the points, choose None from the Style option menu.

To display the line of best fit, select Best fit line. The line is drawn, and the equation of the line and the value of  $R^2$  is displayed in the text box to the right. As well as the line of best fit, you can display the line of perfect correlation or perfect anticorrelation by selecting Diagonal line with slope, and choosing 1 or -1 from the option menu.

### 11.1.3.3 Changing the Axis and Color Scale Settings

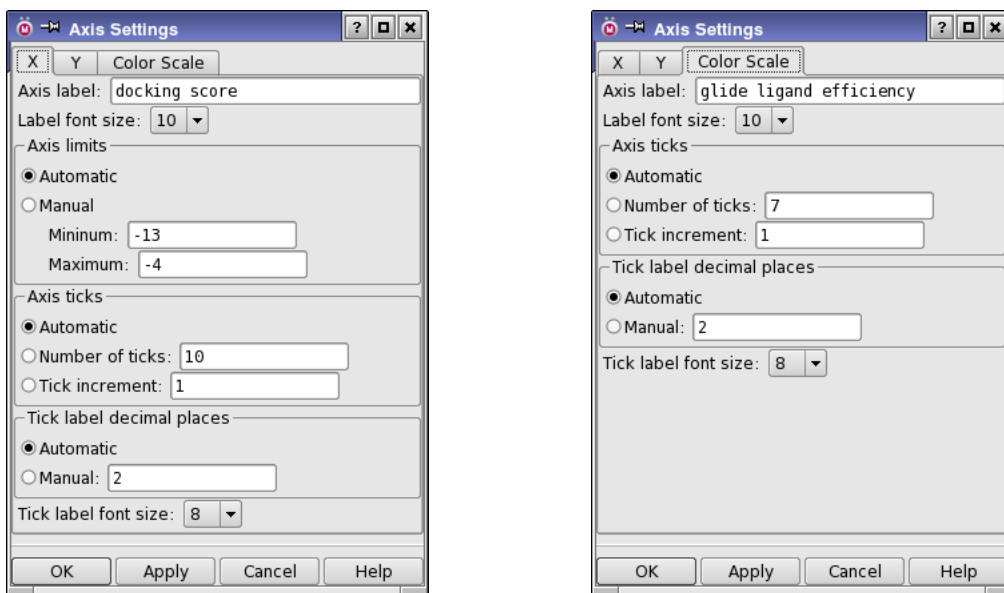
By default, the axes and color scale are labeled with the last selected property, and the axis and color scale range and tick marks are placed automatically. The color scale shows the distribution of colors in the color map. It can be displayed by selecting Color scale.

To change these settings, click Axis Settings, and make the changes in the Axis Settings dialog box. The Axis Settings dialog box has three tabs: X, Y, and Color Scale. These tabs have the same controls, with one exception noted below.

**Axis labels:** To change the label, enter the label to be used for the axis or color bar in the Axis label text box. The default is the property name. To change the font size for the label, choose the point size from the Label font size option menu. The default is 10.

**Axis limits:** In the Axis limits section you can select an option for determining the axis limits. This section is not included in the Color Scale tab. The two options are:

- **Automatic**—Determine the axis limits from the range of values for the axis. Some rounding is done to decrease the number of significant digits in the end points.
- **Manual**—Set the axis limits in the Minimum and Maximum text box. The defaults are the automatically determined limits. If you choose values that are smaller than the actual range, some points will not appear on the plot.



**Figure 11.3.** The X and Color Scale tabs of the Axis Settings dialog box.

You can also enforce the axis ranges to be the same by selecting Equalize axis range in the Scatter Plot panel. This option should only be used when the properties on the two axes have approximately the same range of values, such as in an experimental versus predicted value scatter plot. Otherwise, the plot points will not occupy much of the plot area.

**Axis tick marks:** You can set the number of tick marks on the axis, the number of decimal places used on the numerical labels for the tick marks, and the font size for the tick marks. In the Axis ticks section you can select one of the following options for determining the number of tick marks on the axis:

- **Automatic**—Determine the number of tick marks from the axis range to give a reasonable appearance.
- **Number of ticks**—Specify the number of tick marks to use, including the ends of the range. The axis range is divided by this number minus one to determine the increment.
- **Tick increment**—Specify the increment to use for the tick marks. The number of ticks is determined by the range and the increment.

In the Tick label decimal places section, you can choose from the following options:

- **Automatic**—Determine the number of decimal places from the tick increment.
- **Manual**—Set the number of decimal places in the text box.

The point size for the tick label font can be chosen from the Tick label font size option menu. The default is 8.

#### **11.1.3.4 Changing the Plot Shape and Area**

There are two ways in which you can change the shape of the area used to plot points.

- You can place the axes on the same scale by selecting Equal aspect. The shape of the plot area is changed so that the scales on the axes are the same. This option is useful only when the range of values covered by the axes is approximately the same.
- You can adjust the sides of the plot area by clicking the Configure plot toolbar button.



The Plot Configuration panel opens. In this panel, you can adjust the position of each of the four sides of the plot. To close the panel, use the window controls.

The size and shape of the plot area is also adjusted when you resize the panel or when you hide the controls for the plot.

#### **11.1.3.5 Adding a Title and a Legend**

To add a title above the plot, select Plot Title, and enter the title text in the text box. This title is not the same as the plot name, by which the plot is identified in the project.

To display a legend for the points, which shows the plot symbol for each series and the property chosen for the y axis, choose the legend location from the Legend option menu. The legend is placed inside the plot area.

#### **11.1.3.6 Labeling Plot Points**

You can label the plot points with the value of a property, or view the value of a property for plot points, by using the Label points toolbar button.



When you click this button, a property selector opens, in which you can choose the property that you want to use for the labels or view. Once you have chosen the property, you can view the property value by pausing the pointer over a plot point. The value appears in a tooltip, with an arrow pointing to the point. To label the point with this value, click the point, then move the pointer to the location in the plot area where you want to place the label, and click again. The label moves with its arrow as you move the pointer. To delete the label, click the point again.

You can add labels for multiple properties, but the property name is not included in the label. Only one label can be added to each point.

### 11.1.4 Changing the View of a Plot

The toolbar in the Scatter Plot panel has tools for changing the view of the plot. These tools can be used to pan the plot and zoom in or out. Each time you zoom or pan, the settings for the new view are stored in the view history. You can then step through the different views of the plot, and you can reset the view to the original state. The buttons for the view operations are described below.



#### Reset view

Reset the plot to the original pan and zoom settings.



#### Previous view

Display the previous view of the plot in the view history



#### Next view

Display the next view of the plot in the view history



#### Pan and zoom

Pan the plot with the left mouse button; zoom in and out with the mouse wheel or the right mouse button. Using the mouse wheel preserves the aspect ratio. With the right mouse button, the magnitude of the zoom for each axis is determined by the direction in which you drag.



#### Zoom to rectangle

Drag out a rectangle on the plot to zoom in to that rectangle.

### 11.1.5 Interacting with the Project Table

The toolbar contains buttons for operations on the selected plot that interact with the Project Table: selecting and deselecting entries associated with data points, and including and excluding entries associated with data points. If the Project Table panel is not open, you can open it by clicking the Open Project Table toolbar button:



Clicking the Pick to select entries button enters a mode in which you can select entries in the Project Table by selecting points in the plot.



Clicking the Pick to include entries button enters a mode in which you can include entries in the Project Table by selecting points in the plot.



For both of these modes, you can select points with the following actions:

- Click on a data point to select a single point and deselect all others.
- Shift-click on a data point to add that point to the selection.
- Control-click on a data point to change the selection of that point without affecting the selection of other points.
- Drag over points to select all of those points and deselect all others.
- Hold down SHIFT and drag over points to add points to the selection. Points that are already selected remain selected, so you can drag over a mix of selected and unselected points to add the latter to the selection.
- Hold down CTRL and drag over points to change their selection without affecting the selection of other points. When you do this, the points in the region you drag out that were already selected are deselected, and the points that were not selected are selected.
- Click in a blank area of the plot to clear the selection of points.

### 11.1.6 Saving Plot Images

You can save an image of the plot area with the Save plot image toolbar button.



When you click this button, a file selector opens, in which you can choose the image format, navigate to the desired location, and name and save the file.

## 11.2 Plotting Coordinate Scan Results

You can display the results of a scan of one or two coordinates in the Plot of One-Coordinate Scan panel or the Plot of Two-Coordinate Scan panel in Maestro. Scans can be generated by MacroModel or Jaguar. The data from these scans is stored in .grd files, which must be opened from the panel. To open a .grd file, click the Open button, navigate to the file, select it, and click Open. The panels and their use is described below. Since there are many common features of these panels, the general features are described first.

To open the Plot of One-Coordinate Scan panel, choose Tools → Plot Coordinate Scan → One Coordinate. To open the Plot of Two-Coordinate Scan panel, choose Tools → Plot Coordinate Scan → Two Coordinates.

### 11.2.1 General Features of Coordinate Scan Plot Panels

Each panel consists of a toolbar, a plot area on the right and a set of controls on the left. The common controls are described below; the controls specific to a given plot are described in later sections.

Minimum energy, Maximum energy

These text boxes allow you to set the energy range for the plot.

Full Scale

Restores a plot whose range has been altered to its full scale.

Energy Units

These options allow you to display data in either kJ/mol or kcal/mol energy units.

Energy Scale

These options allow you to display the energy as either an absolute or a relative value. The Relative option is useful for estimating rotational barriers.

Show legend

Show a legend for the plot.

Decimal places

Specify the number of decimal places to be displayed for the values on the  $x$  and  $y$  axes.

The panel has a toolbar that you can use to configure the plot or to save an image of the plot. The toolbar buttons are described below.



Reset

Reset the plot to the original pan and zoom settings.



Back

Display the previous view of the plot in the view history



Next

Display the next view of the plot in the view history



### Pan/zoom

Pan the plot by dragging with the left mouse button, zoom by dragging with the right mouse button.



### Zoom to rectangle

Drag out a rectangle on the plot to zoom in to that rectangle.



### Configure subplots

Configure the margins and spacing of each plot in the panel.



### Edit axis and curve parameters

Make settings for the title, range, labeling, and scale of the axes; the color, style, and width of lines; and the color, style, and size of markers.



### Save image

Save an image of the plot to file. Opens a file selector in which you can browse to a location, select the image format, and name the image.



### Copy to clipboard

Copy an image of the plot to the clipboard. You can then paste it into another application. This button is only available in some panels.

## 11.2.2 The Plot of One-Coordinate Scan Panel

After a scan calculation with a single geometric parameter has been successfully completed, the resulting `.grd` file can be displayed graphically using this panel. To open a `.grd` file, click the Open button, navigate to the file, select it, and click Open. The data from the `.grd` file is displayed in the plot area. The corresponding structures are read into Maestro as a scratch entry, and one of the structures is displayed in the Workspace.

The appearance of a displayed plot can be changed using the controls on the left side of the panel and the controls in the Plot Settings - One-Coordinate Scan panel, which is opened by the Plot Settings button.

- The ranges of the axes can be changed by entering values in the Minimum coordinate, Maximum coordinate, Minimum energy and Maximum energy text boxes.
- The symbol shape, color, and size and the curve style, color, and width are all controlled from the Plot Settings - One-Coordinate Scan panel. To change these attributes, select the data set in the list at the top of the panel, then choose the attributes from the option menus.

You can display multiple plots from `.grd` files in the Plot of One-Coordinate Scan panel. Each plot is added by clicking the Open button and selecting the `.grd` file. The data sets are listed in the Plot Settings - One-Coordinate Scan panel. You can delete a plot by selecting it in the list and clicking Delete.



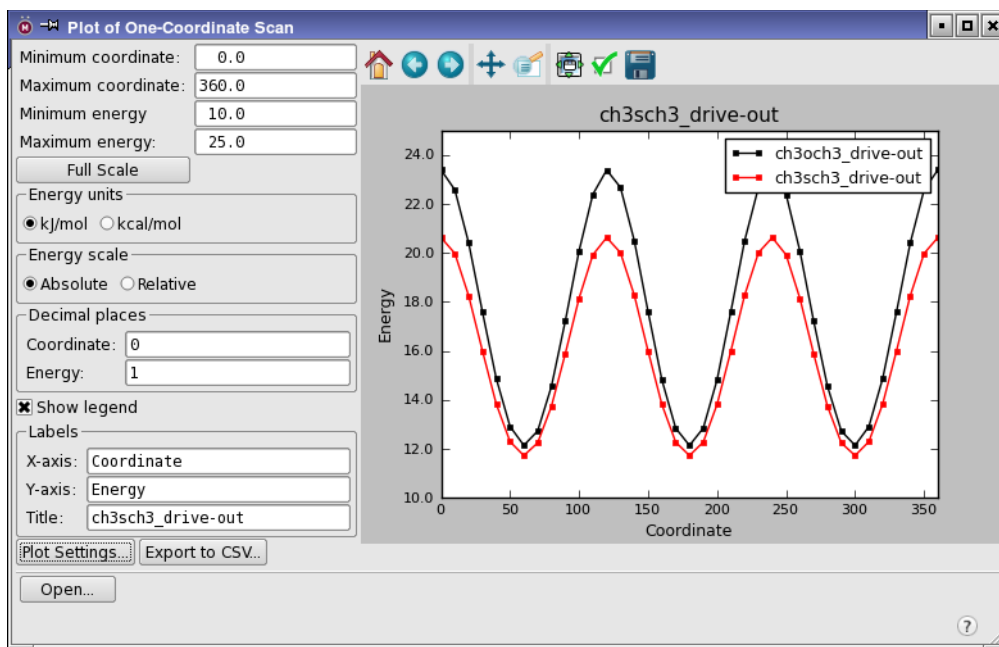


Figure 11.4. The Plot of One-Coordinate Scan panel.

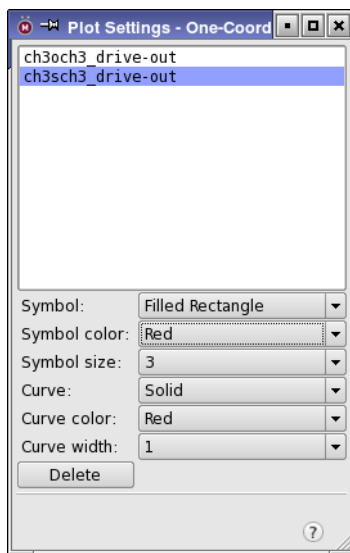


Figure 11.5. The Plot Settings - One-Coordinate Scan panel.

To create a comma-separated file that can be read by a spreadsheet, click **Export to CSV**. A file selector opens, in which you can navigate to a location and name the file. The data for all available plots is written to this file.

### 11.2.3 The Plot of Two-Coordinate Scan Panel

For two-dimensional scans, the data from the `.grd` file is displayed in the plot area as a contour map. Only one `.grd` file can be displayed at any given time. Reading in a second file clears the data from the first.

The appearance of a displayed plot can be changed using the controls on the left side of the panel. You can set the number of contour lines with the **Number of Contours** option menu, the line thickness with the **Contour Width** option menu, and use dashed lines for negative contour values by selecting **Negative Dashed**. You can choose the color map used to display the contours from the **Color map** option menu. You cannot, however, change the range of coordinates displayed.

To determine the contour intervals, Maestro divides the range of energy values specified in the **Minimum Energy** and **Maximum Energy** text boxes (or the maximum and minimum values in the file) by  $n+1$ , where  $n$  is the specified number of contour lines. This means that the maximum and minimum energy values are not represented by contour lines.

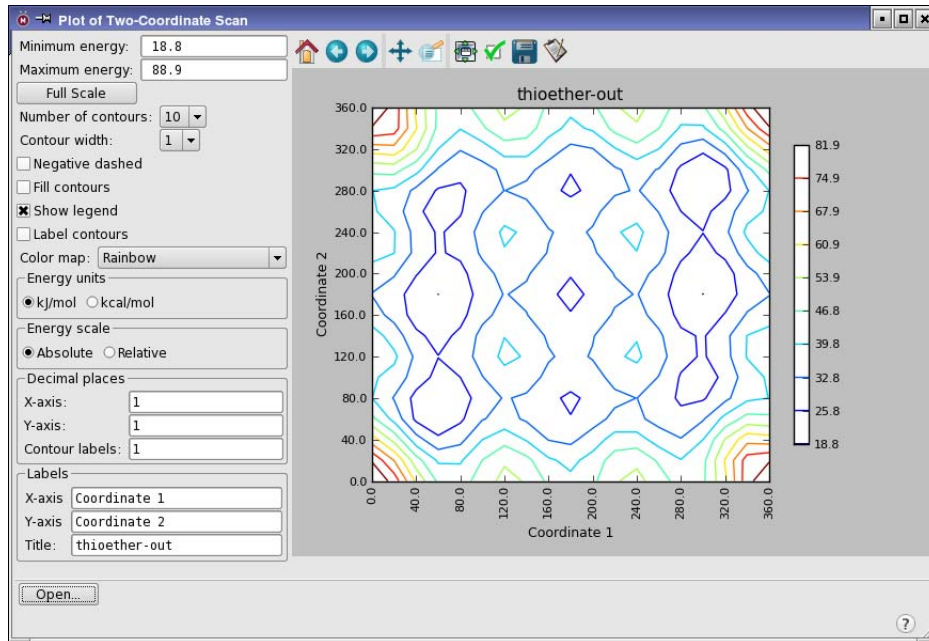


Figure 11.6. The Plot of Two-Coordinate Scan panel.

# Surfaces

The Maestro surface facility allows you to create and visualize molecular structure surfaces, extended radius surfaces, van der Waals surfaces, electrostatic potential surfaces, and maps of active sites in receptor molecules; to import surfaces; to display crystallographic density maps; and to display surfaces generated by Jaguar, QSite and the Semiempirical NDDO package, such as electrostatic potential surfaces, density surfaces, and molecular orbitals.

Some surfaces are constructed directly as a set of surface elements. Other surfaces are derived from data for a function on a three-dimensional grid. This data is called a *volume*. The surface is created by selecting a value for the function and displaying the surface that corresponds to that value. The value is called an *isovalue*, and the surface is called an *isosurface*. Volumes can also be rendered as a function of the data value in the Workspace by defining a map of the data values to the opacity and to color ramps.

Generated surfaces are incorporated into the Project Table and are displayed in the Workspace by default when the associated entry is included. Surface data for any entry can be viewed using the Manage Surfaces panel. From this panel, you can change surface display properties, such as transparency, display style, and color, and edit the volume map.

## 12.1 Generating Surfaces

From the Surface submenu of the Workspace menu in the main menu bar, you can generate three kinds of surfaces that have similar characteristics: molecular surfaces (Connolly surfaces), van der Waals surfaces, and extended radius surfaces. The panels for these surfaces are docked into the Workspace by default.

Surfaces can only be generated for project entries. If you try to generate a surface for the scratch entry, you will be prompted to create a project entry from the scratch entry. Each surface is associated with only one entry, but an entry may have zero or more surfaces.

### 12.1.1 Surface Generation Controls

Most of the surface-generation settings are common to the Molecular Surface panel, the Extended Radius Surface panel, and the VDW Surface panel. All the settings are discussed below.

### Atoms for surface display

The surface is displayed only for the atoms specified in the Atoms for surface display section of the panel. You can select atoms by picking in the Workspace, by entering an ASL expression in the ASL text box, by clicking All, or by clicking the Atom Selection button and choosing an atom selection item or clicking Select to open the Atom Selection dialog box. If you want to reset the atom selection, click the Clear button. If you have Markers selected, the atoms you select are marked in the Workspace.

### Boolean operation

In the Molecular Surface panel, you can create surfaces that are formed by Boolean operations on two surfaces. The operations are:

- None—Create a single surface. This is the default.
- Union—Create a surface that encloses the volume occupied by either of the two surfaces (Boolean OR).
- Intersection—Create a surface that encloses the common volume of the two surfaces (Boolean AND).
- Difference—Create a surface that encloses the volumes that are unique to each surface (Boolean XOR).

The atoms for the second surface are specified in the Atoms for surface boolean operation section, which is displayed when you choose an operation other than None. The controls are the same as in the Atoms for surface display section.

### Surface context

The surface is actually generated for the atoms chosen from the Surface context option menu, but only the portion of the surface defined by the Atoms for surface display is displayed. If you choose Entry or Molecule, the surface is generated for the entries or molecules of which the atoms selected for surface display are a part. If you choose Selected atoms, the surface is generated only for the atoms selected for surface display, and appears as a complete surface.

You can also limit the surface dynamically once it is created, using the Limit Surface dialog box. See [Section 12.4.1 on page 306](#) for details.

### Surface resolution

You can set the quality of the image to Low, Medium, or High with this option menu. These controls set the grid spacing for surface generation. You can also choose Custom and enter a grid spacing in the text box. The grid spacing values for the other three choices are displayed in this text box. The high quality surface is smoother but takes longer to generate.

### Probe radius

This setting appears only on the Molecular Surface panel and the Extended Radius Surface panel. Since the van der Waals surface is, by definition, built directly on the van der Waals spheres, a probe radius setting is not needed for this panel.

The value in the Probe radius text box controls the radius of the probe sphere that is “rolled over” the van der Waals surface of the molecule. The default probe radius of 1.4 Å corresponds to water.

### VDW radius scale

This setting allows you to scale the van der Waals radius before the probe is used to generate the surface.

### Create Surface

To start the surface generation, click Create Surface. During this time Maestro is inoperative and no user interaction is possible. For large surfaces and high quality, surface generation can be time consuming.

## 12.1.2 Molecular Surfaces

In the Molecular Surface panel, you can generate a surface that follows the molecular surface, but is smoother than the CPK surface. The best known type of molecular surface is the Connolly surface. Imagine rolling a ball, representing a solvent molecule, over the assembly of spheres constituting the van der Waals surface. Where the outside of the ball contacts the van der Waals spheres, the surfaces coincide. Where two van der Waals spheres intersect, the Connolly surface follows the surface of the solvent sphere, producing fillets rather than cusps.

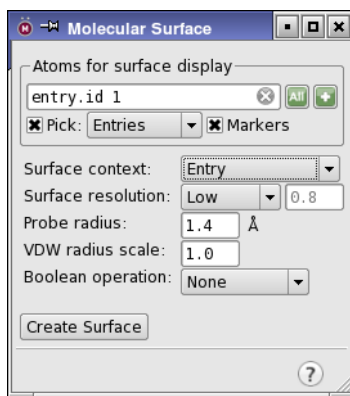


Figure 12.1. The Molecular Surface panel.

Changing the solvent sphere (probe radius) affects the size and shape of the surface. Reducing the grid spacing improves the accuracy of the surface, but increases the calculation time.

You can also generate a surface by performing a Boolean operation on two surfaces—see the previous section for details on how to do this.

To open the Molecular Surface panel, choose *Workspace* → *Surface* → *Molecular Surface*. Instructions for using the settings in the Molecular Surface panel are described in [Section 12.1.1 on page 295](#). The default surface context is *Selected atoms*.

When you display a molecular surface, the surface color can be darkened according to cavity depth. This feature highlights the shape of the surface, providing an effect similar to shadows. You can turn this effect on or off with the *Darken colors by cavity depth* option, under *Surfaces – Appearance* in the Preferences panel.

### 12.1.3 Extended Radius Surfaces

In the Extended Radius Surface panel, you can generate a surface constructed on van der Waals spheres in a similar way to a Connolly surface. In an extended radius surface, the point that corresponds to the center of the probe is used to generate the surface, rather than the point representing the closest contact of the probe with the surface. An extended radius surface therefore shows roughly the surface that the centroid of a solvent or a ligand cannot penetrate. Thus, looking at bound ligands with wire bond representation, the ligands would “hug” but not penetrate the extended-radius surface.

To open the Extended Radius Surface panel, choose *Workspace* → *Surface* → *Extended Radius*. Instructions for using the settings in the Extended Radius Surface panel are described in [Section 12.1.1 on page 295](#).

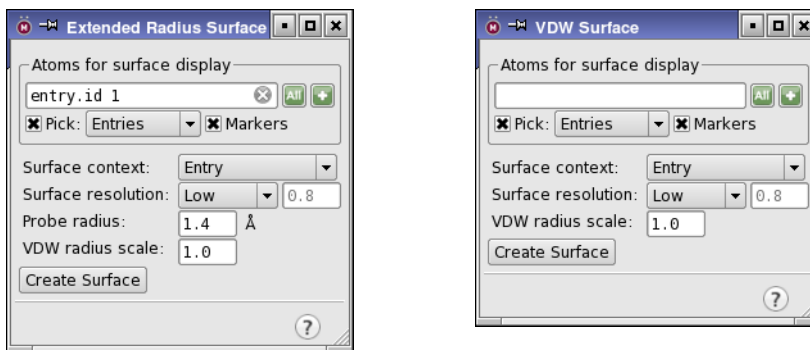


Figure 12.2. The Extended Radius Surface panel (left) and the VDW Surface panel (right).

### 12.1.4 Van der Waals Surfaces

The VDW Surface panel is used to generate a van der Waals surface. This surface is identical to the CPK molecular representation with the percentage set to 100.

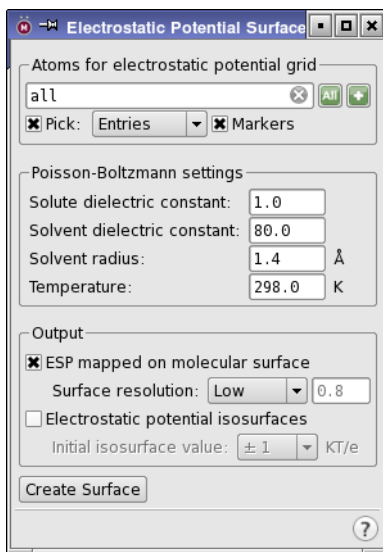
To open the VDW Surface panel, choose *Workspace* → *Surface* → *Van der Waals*. Instructions for using the settings in the VDW Surface panel are described in [Section 12.1.1 on page 295](#).

### 12.1.5 Electrostatic Potential Surfaces

The Electrostatic Potential panel is used to generate a volume that contains values of the electrostatic potential. To open the Electrostatic Potential panel, choose *Workspace* → *Surface* → *Poisson-Boltzmann Electrostatic*.

The electrostatic potential is derived from the partial atomic charges by solving the Poisson-Boltzmann equation on a 3D grid of points, and is evaluated with a continuum solvation model. By default, the calculation is done for the entire *Workspace*, but you can limit it to the region around a particular set of atoms (for example, a ligand in a complex), by selecting the atoms with the *Atoms for electrostatic potential grid* picking tools. If you limit the grid, the electrostatic potential is still evaluated with respect to the entire *Workspace*, but is only represented on the grid you define.

Some of the parameters for the Poisson-Boltzmann solver can be set. You can change the internal dielectric constant of the solute, and you can set the dielectric constant and radius of



**Figure 12.3.** The Electrostatic Potential Surface panel.

the solvent. The default values are set for water. You can run the calculation at different temperatures.

The output from this panel can be mapped onto a molecular surface (which is generated if this feature is requested), and it can be represented as a pair of isosurfaces, one for each sign of the potential. If you choose to map onto a molecular surface, the same image quality controls as in the Molecular Surface panel are available. The color scheme for the surface mapping can be set in the Surface Display Options dialog box. If you choose to create isosurfaces, you can set the initial isosurface value. Using the isosurfaces is a way to identify regions of large positive or negative electrostatic potential.

Electrostatic potential surfaces can also be generated by Jaguar, from the electron density. See Section 3.10 of the *Jaguar User Manual* for details.

## 12.2 Hydrophobic/philic Surfaces

Maestro provides a tool that is designed to help you to visualize the preferred locations of ligand atoms in a receptor site. Using the Hydrophobic/philic Surfaces panel, you can generate a surface that displays hydrophobic and hydrophilic regions within the active site of a protein. To open the Hydrophobic/philic Surfaces panel, choose Hydrophobic/philic from the Surface submenu of the Workspace menu.

### 12.2.1 Background

Given a receptor structure, the accessible space in the active site is partitioned into three types of regions:

1. **Hydrophobic**—regions that are favorable for occupancy by hydrophobic ligand groups

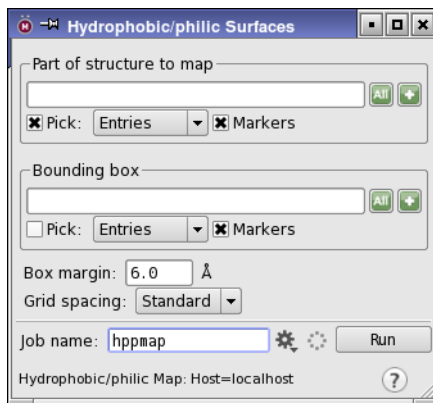


Figure 12.4. The Hydrophobic/philic Surfaces panel.



2. **Hydrophilic**—regions that are favorable for occupancy by hydrophilic ligand groups
3. **Neither hydrophobic nor hydrophilic**—regions that are of mixed character or that are far enough from the receptor surface to be similar to bulk water, where to a first approximation any group could reside with little effect on the binding affinity.

Hydrophobic and hydrophilic regions are marked by surface contours that enclose the region. The “neither” regions are implicit; these are simply regions that are accessible to the ligand but are not marked as being either hydrophobic or hydrophilic.

By revealing “targets of opportunity”—e.g., hydrophobic regions that have room to accommodate a larger hydrophobic group—active site maps can aid in the design of new ligands. Alternatively, by showing the degree to which poses produced by a program like Glide display or violate proper complementarity to the receptor site, site maps can aid in the evaluation of docking hits. The “neither” regions are also important because they are regions in which the physical properties of the ligand can be changed, for example to make the ligand more or less soluble, with minimal expected effect on the binding affinity.

The active-site mapping procedure operates in a manner analogous to Goodford’s GRID algorithm (P. Goodford, *J. Med. Chem.* **1985**, 28, 849). Hydrophilic and hydrophobic regions are defined in a way that considers both spatial proximity to the receptor and suitability for occupancy by solvent water. A putative van der Waals energy and the magnitude and direction of the electric field (calculated using a distance-dependent dielectric formulation) are computed for a probe centered at each grid point by considering interactions with all atoms of the receptor site within a defined cutoff distance. In contrast to techniques that color-code the receptor surface to represent hydrophilicity or hydrophobicity, these maps depend on more than the character of the nearest receptor atom. Moreover, the maps explicitly show the shape and extent of hydrophilic and hydrophobic regions, something a receptor-surface display cannot do. The maps behave rather like an “extraradius” surface in that the atoms of a wire frame representation of the ligand can approach but should not penetrate the map surface (except in hydrogen bonding regions, where internuclear distances are expected to be smaller than normal contact van der Waals distances).

**Hydrophilic Map:** The hydrophilicity is defined by adding an “electric-field reward” term to the vdW energy:

$$\text{Grid\_philic} = \text{vdW\_energy} + \text{oriented-dipole\_energy} \quad (1)$$

where the oriented-dipole energy is necessarily negative. Hydrophilic regions are those within which the sum of the two terms is sufficiently negative, and are displayed by contouring the hydrophilic grid at a prescribed negative isovalue, typically  $-6 \text{ kcal mol}^{-1}$ .

**Hydrophobic Map:** The quantity representing hydrophobicity is constructed by adding an oppositely signed (positive) “electric-field penalty” term to the vdW term:

$$\text{Grid\_phobic} = \text{vdW\_energy} - 0.15 * \text{oriented-dipole\_energy} \quad (2)$$

Hydrophobic regions are those for which the favorable van der Waals term is not too strongly degraded by the positive electric-field penalty. Qualitatively, hydrophobic regions are those that lie suitably close to the surface of the receptor but for which the water-dipole-orienting electric field produced by the receptor is sufficiently small. In short, these are regions where something would like to be, but water would not. Hydrophobic regions are displayed by contouring the hydrophobic grid at a suitably negative isovalue, typically  $-0.5 \text{ kcal mol}^{-1}$ .

### 12.2.2 Mapping Algorithm

The first step is to define a rectilinear box that contains an active site and to define grid points with a typical grid spacing of  $1 \text{ \AA}$  within the box.

Next, van der Waals energies and  $x$ ,  $y$ , and  $z$  electrostatic field components are computed at each of the grid points. Receptor atom partial charges and van der Waals parameters are taken from the OPLS-AA force field. A probe is represented by a van der Waals sphere of radius  $1.5 \text{ \AA}$ , well depth  $0.2 \text{ kcal mol}^{-1}$ , and point dipole moment  $2.3 \text{ Debye}$ . The probe’s point dipole is oriented along the electric field to give a minimum (negative) electrostatic energy and is offset from the vdW body (which is located at the grid point and represents the oxygen atom of a water molecule) toward the center of an optimally oriented O–H bond. A smoothing procedure is applied during the calculation of the receptor’s electric field to avoid artificial singularities. The hydrophilic and hydrophobic grid values are then determined from Eqs. 1 and 2.

Finally, the hydrophilic and hydrophobic grids are read by Maestro, which contours the grids at the empirically selected default isovalues cited above ( $-6$  and  $-0.5 \text{ kcal mol}^{-1}$ ) and displays the corresponding hydrophilic and hydrophobic volumes as surfaces.

### 12.2.3 Specifying a Structure to Be Mapped

To create a map of a receptor structure, you must first include the structure in the Workspace. The structure must belong to an entry in the current project: you cannot map structures from more than one entry or from a scratch entry.

Once you have displayed the structure, specify the part of the structure to be mapped with the tools in the Part of structure to map section. You can pick atoms in the Workspace, enter an ASL expression, click All, or click the Atom Selection button to choose from a range of predefined atom groups or open the Atom Selection dialog box and select atoms. If Markers is selected, a dark pink trace is superimposed on the selected atoms and bonds.

To clear the atom selection, click the Clear button. Clearing the selection does not delete existing maps.

### 12.2.4 Defining the Mapping Box

In addition to specifying the structure for which a map is to be generated, you must also set the location and size of the “box” of atoms to be mapped, using the tools in the Bounding Box section. You can pick atoms in the Workspace, enter an ASL expression, click All, or click Select to open the Atom Selection dialog box and select atoms. Mapping box atoms must be associated with a project entry; they cannot be part of the scratch entry. If Markers is selected, an orange box is displayed in the Workspace to mark the mapping box region.

The box margin provides a buffer around the minimal defined mapping box enclosure. Adding a buffer region may be useful if you are investigating modification of the ligand to obtain a better fit in the active site, and would like to generate a surface large enough to show how modified or added atoms would interact.

To alter the box margin, enter a value into the Box Margin text box. If you have defined the mapping box region using `fillres` in an ASL expression, you may want to set the box margin value to zero.

### 12.2.5 Running the Job

In contrast to the generation of other types of surfaces, mapping of an active site is run as a job. After you have configured the Hydrophobic/philic Map panel settings, you can choose to either run the job or to simply write out the job files so that you can run the calculation later.

To write the job files without running the job, click the Write button. You can use these files to subsequently launch the calculation from the command line.

To set up and run the calculation, click Start, make settings in the Start dialog box, and click Start to launch the job. This job is *not* run at reduced priority if it is run locally, unlike most local jobs.

When the job finishes, the surface data is incorporated into the project and an S button is added to the Title column for the entry, which you can click to open the Manage Surfaces panel and view the data associated with this surface.

### 12.2.6 Viewing the Surface

The site map is displayed as a pair of isosurfaces generated from the hydrophilic and hydrophobic grids. The default isovalues can be changed in the Surfaces panel if more expansive or more restrictive philic and phobic volumes are appropriate in a given application. If you need

to see inside these surfaces, you can display them as Mesh surfaces, or if you display them as Solid surfaces (the default), you can increase the transparency.

## 12.3 Importing Surface or Volume Files

You can import surfaces or volumes from one or more files into the Maestro project and associate these surfaces or volumes with a project entry. The file formats that are recognized by Maestro are given in [Table 12.1](#).

To import a file, choose Display → Surface → Import, or click the Import button in the Manage Surfaces panel. Browse for the desired files and click Import. The data must be associated with a project entry, so once you have selected the files, the Choose Entry dialog box opens. In this dialog box, choose the entry to which the surface or volume data belong. Once you have associated the data, it becomes a part of the Maestro project. It can be displayed by clicking the S button in the Title column of the Project Table or by clicking in the In column of the surface table in the Manage Surfaces panel.

*Table 12.1. Surface file formats.*

File Extension	Format description
.vis	Schrödinger format. Files in this format are created by Jaguar, QSite, Semiempirical NDDO, SiteMap, and hppmap.
.plt	Obsolete Jaguar format.
.cns, .map	CNS electron density map format. Used by PrimeX.
.ccp4	CCP4 electron density map format. Used by PrimeX.

If you are importing an electron density map, the Map Type dialog box is displayed after choosing the entry, so that you can select the map type from among the common types. Selecting the map type is important for PrimeX operations that expect a particular type of map.

When you import surface or volume files, the surfaces and volumes are already named. To change the name of the displayed surface or volume, edit the name in the Surface Name field in the surfaces table.

A .vis file can contain volumes, surfaces, or both. A volume contains all of the data values for each of the points on the grid. Once the file is imported into Maestro, one or more surfaces can be created. In addition, if the .vis file still contains the original volume data used to generate an imported surface, you can change the isovalue in Maestro and generate new surfaces using different isovalues. If a Maestro .vis file contains only surfaces, then it contains only a description of the surface and not the original volume data from which it came. You cannot change the isovalue for such a surface in Maestro.

Jaguar-generated `.vis` files always contain volume data—3D grids with data values at each point. They may contain orbital, electron density, spin density, or electrostatic potential information. These files are created using the appropriate keywords in the **gen** section in the Jaguar input file. See [Section 3.10](#) of the *Jaguar User Manual* for details. Likewise, surfaces generated by SiteMap, WaterMap, and hydrophobic/philic maps contain volume data. The surface and volume data from all these applications is automatically incorporated into the project and displayed.

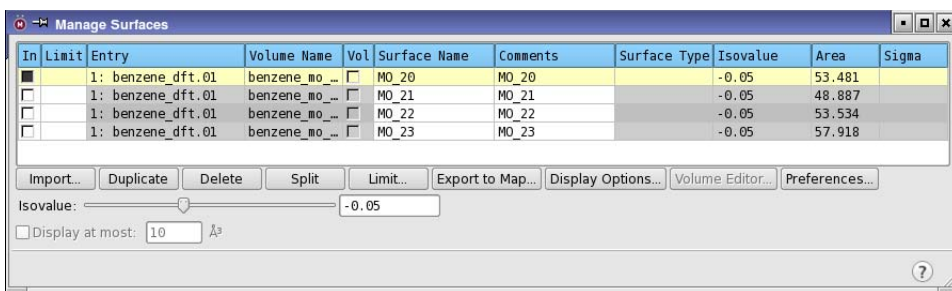
## 12.4 The Manage Surfaces Panel

The Manage Surfaces panel is used to import, modify, and view surfaces and their properties. The panel consists of a table of surfaces for all entries that are included in the Workspace, and a set of controls below the table. The columns of the surface table are described in [Table 12.2](#). Scratch entries are not part of a project and thus cannot be used for surfaces.

To open the Manage Surfaces panel, choose `Workspace → Surface → Manage Surfaces`, or click the S button in the Title column of the Project Table panel.

*Table 12.2. Surface table columns.*

Column	Purpose
In	Displays or undisplay the surface for that entry in the Workspace.
Limit	If limits are set for this entry, a checkbox appears. You can then check or uncheck the box to turn limits on or off. To add or edit limits, click the Limit button.
Entry	Lists the entry ID and the title of the entry that contains the surface.
Volume Name	Lists the name of the volume from which the isosurface was created.
Vol	Displays or undisplay the volume for that entry in the Workspace.
Surface Name	Edit this field to create a unique surface name within each entry.
Comments	Edit this field to add your own comments. Jaguar fills this field in with molecular orbital names.
Surface Type	Lists the type of surface to be displayed: molecular surface, Van der Waals, extended radius, density, potential, orbital, spin, hydrophobic, or hydrophilic.
Isovalue	Lists the value that was used to create the surface. To change this value, use the Isovalue slider at the bottom of the panel or enter a value in the text box next to it. For regular surfaces, this field is blank.
Area	Lists the surface area of the limited surface (summation of all polygons).
Sigma	(PrimeX only) Sigma value used to generate the map.



**Figure 12.5. The Manage Surfaces panel.**

- To display a single surface in the Workspace, click in the In column for the desired surface.
- To display multiple surfaces, click the first and shift-click the last in the In column.
- To display or undisplay individual surfaces, use control-click or middle-click in the In column.
- To change the name of a surface, enter a new name in the Surface Name column
- To arrange the surfaces in a rectangular grid, choose View → Tile → Tile by Surface followed by View → Tile Workspace (or use the Tile button on the View toolbar).

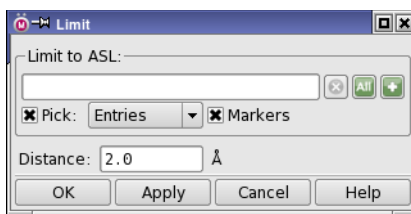


Below the table are buttons for importing, duplicating, deleting, and limiting surfaces, as well as controlling the display of surfaces and volumes and for setting surface-related preferences. You can adjust the isovalue of a volume with the slider or the text box. These controls and buttons are described in the following sections.

### 12.4.1 Importing, Modifying, and Deleting Surfaces

#### Importing surfaces

You can import surfaces from a file into the Manage Surfaces panel. To do so, click Import, browse to select the desired surface file, and click Import. You can also import surfaces by choosing Workspace → Surface → Import in the main window. More information is given in [Section 12.3 on page 304](#).



**Figure 12.6. The Limit panel.**

### Changing isovalues

The isovalue is the current value of the property that was used to create the surface. Surfaces generated by Jaguar and hydrophilic/phobic surfaces have volume data for which an isovalue is specified. Molecular surfaces, van der Waals surfaces, and extended radius surfaces do not have volume data.

You can change the isovalue for a surface that has an associated volume: either enter a new number in the Isovvalue text box at the bottom of the panel or use the slider to adjust the isovalue. The surface is redisplayed with the new isovalue. For PrimeX, the fraction of Sigma is also displayed.

To create a new isovalue for a surface, select the surface in the table and click the Duplicate button at the bottom of the panel. Then you can change the isovalue for the new surface.

### Limiting the display volume of surfaces

You can limit the visible portion of the surface to the portion that is within a specified distance from a selection of atoms. Click Limit to open the Limit panel. Select the atoms using the picking tools in the Limit to ASL section, enter a value in the Distance text box, and click Apply. The limit is applied to the surface. You can change the atom selection, or click OK to accept the limit. To remove the limit, click the square in the Limit column of the surfaces table.

You can also limit surfaces by only displaying the surface within a cube of a specified volume. To do so, select Display at most, and enter a volume in the text box.

### Splitting paired surfaces

Surfaces calculated from volume data that have both positive and negative values are displayed as paired surfaces: one for the positive values and one for the negative values. Examples of such surfaces are molecular orbitals, electrostatic potentials, and crystallographic density difference maps (Fo-Fc). You can display just the positive or the negative surface, by selecting the surface in the table and clicking Split. Two new surfaces are created, one for the positive surface and one for the negative surface, with suffixes `_positive` and `_negative`.

## Deleting surfaces

To delete a surface, select it in the surfaces table and click Delete.

## 12.4.2 Changing the Appearance of the Surface

You can adjust various characteristics of the surface's appearance using the controls in the Surface Display Options dialog box. Many of these controls are available from the shortcut menu, which opens when you right-click on a row in the table. This menu allows you to change the style and transparency, and color with a constant color or by the value of a property.

In addition, there are preferences for the display of surfaces that can be set in the Surfaces tab of the Preferences panel—see [Section 14.9 on page 361](#) for details.

### 12.4.2.1 Style and Transparency

Surfaces can be displayed in three styles: Solid, Mesh, and Dot. The transparency of Solid surfaces can be changed using the Transparency sliders. Mesh and Dot surfaces are opaque unless the Transparency slider is set to 100%, when they become invisible.

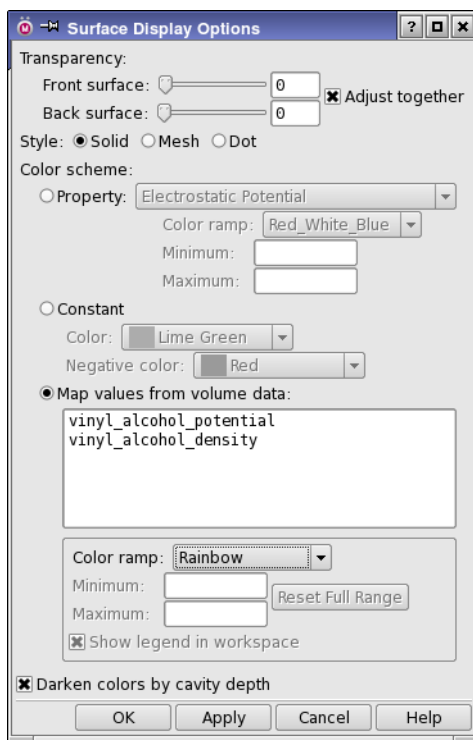


Figure 12.7. The Surface Display Options dialog box.



You can adjust the transparency of the front and back of the surface independently, with the Front surface and Back surface sliders and text boxes. By default, these controls are linked. To allow them to be adjusted independently, deselect Adjust together. The default values of the transparency can be set in the Surfaces tab of the Preferences panel.

You can also use the shortcut menu to choose from several preset transparency values: 0%, 25%, 50%, and 75% transparency for both front and back, and Front Face 100% (with 0% for the back), which makes the front face completely transparent.

The transparency can be made to vary across the surface, according to the angle the surface normal makes with the plane of the screen. The transparency is a minimum when the normal is perpendicular to the screen, and a maximum when it is parallel to the screen. This gives an effect like looking through a balloon, where the color is darker toward the edges of the view and lighter in the middle. This effect is controlled by the Angle-dependent transparency preference, under Surfaces – Viewing in the Preferences panel—see [Section 14.9.1 on page 361](#). The transparency slider in the Surface Display Options panel controls the maximum transparency used.

**Note:** Angle-dependent transparency is only available with an OpenGL graphics level of 2.1.

#### 12.4.2.2 Color Scheme

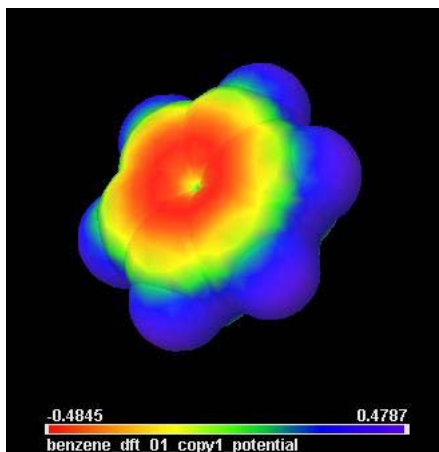
You can color a surface using the following options in the Color Scheme section of the panel:

- **Property**—each part of the surface is colored according to the value of the property on the nearest atom to that part of the surface. Choose a property from the Property option menu. The properties include such things as Entry and Molecule Number, as well as numerical properties like Electrostatic Potential and Residue Charge. Atom Color and CA Atom Color use the color of these atoms to color the surface.

The Partial Charge and Electrostatic Potential schemes require partial charges, which you can generate with a MacroModel, Impact, Prime, or Jaguar calculation. You can also generate partial charges by choosing Assign Partial Charges from the Tools menu. If partial charges are not available, the surface appears completely white.

For the Electrostatic Potential color scheme, you can choose a color ramp from the Color ramp option menu. By default, the range of colors is determined by the range of property values. You can set minimum and maximum property values for the ends of the color ramp in the Minimum and Maximum text boxes. The colors for property values outside the minimum and maximum are set to the colors at the appropriate end of the ramp.

- **Constant**—the entire surface is colored with the same color, which you can choose from the Color option menu. You can make this the default surface color by clicking Set Default Color.



**Figure 12.8. Example of color ramp: electrostatic potential of benzene from Jaguar mapped to van der Waals surface.**

When a surface has both positive and negative portions (a “split” surface, such as a molecular orbital), the **Negative color** option menu is active and you can select the color in which the negative surface is displayed.

- Map values from volume data—the surface is colored based on the value of the volume on the surface, which you select in the list.

The color fades between the colors selected in the **Color ramp** option menu according to the value of the volume property on the surface. By default, the range of colors is determined by the range of values in the volume. You can set the minimum and maximum volume property values represented by the color ramp in the **Minimum** and **Maximum** text boxes, and revert to the default by clicking **Reset Full Range**. You can also display a legend in the **Workspace** that shows the color ramp and value range used. The legend is labeled with the volume name.

This scheme can be used, for example, to display the values of the electrostatic potential obtained from a Jaguar calculation on the van der Waals surface, as shown in [Figure 12.8](#). You can also create your own color ramp (see [Section 13.5.4](#) on [page 323](#) for instructions).

### 12.4.2.3 Depth Perception

If you want to enhance the perception of the depth of the cavities in a surface, select **Darken colors by cavity depth**. This option determines the depth of a cavity in the surface relative to a smooth surface that covers the cavity, and changes the color shade according to the depth of the cavity. For new surfaces, this option is set by a preference—see [Section 14.9.1](#) on [page 361](#).

Another depth perception feature is the use of depth-enhancing contours, which are outlines on the surface that are drawn when the features behind it are more than a certain distance away. This feature, including controls for the distance, the thickness of the contour, and the blending with the background, is available in the Preferences panel—see [Section 14.9.1 on page 361](#).

### 12.4.3 Displaying Volumes

Volume data can be displayed as a continuous function of the data value, rather than just at a particular value (the isovalue). The display is created by setting the opacity and the color of the surface as a function of the data values. To display a volume in this way, select its Vol column.

The function is set up graphically in the Volume Color Map Editor panel, which you open by clicking Volume Editor.

The opacity and color are set up in a graphical manner, by adding points to the opacity chart at particular values of the property and the opacity, and with a particular color value. These points can be dragged around to change the shape of the opacity curve. The color is interpolated linearly between points, and the logarithm of the opacity is interpolated linearly between points. You can also define “peaks” which consist of a point at some opacity and property value, and two points on either side at zero opacity. Peaks can be moved and their width changed. An initial curve is loaded when you open the editor for a particular volume, taken from information stored with the volume.

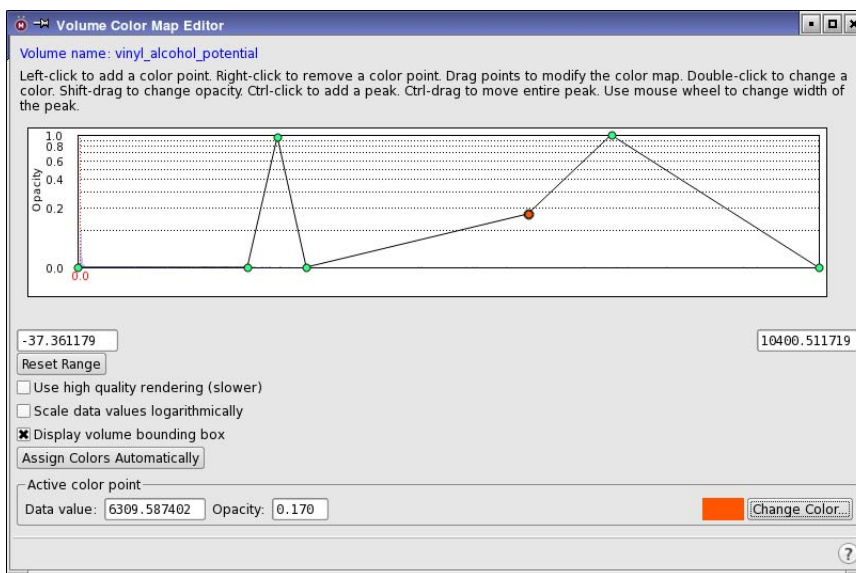
The basic actions for defining the points are as follows:

- To add a point: click on the chart.
- To remove a point: right-click on the point.
- To move a point: drag it to its new location.
- To move a point vertically: shift-drag it to its new location.
- To change the color: double-click on a point.
- To add a peak: control-click on the chart.
- To move a peak: control-drag it to its new location.
- To change a peak width: use the scroll wheel; add SHIFT for finer control.

For detailed control, you can use the Active color point section to change the data value, the opacity, and the color for the current point.

You can change the range of values used in the map by editing the text boxes for the minimum and maximum values. To reset the range to the default, click **Reset Range**.

If the data values span many orders of magnitude, and the details of interest occur at different orders, you can use the logarithm of the data values rather than the values themselves. The data values should all have the same sign. An example is the electron density.



**Figure 12.9.** The Volume Color Map Editor panel.

The panel also has some display options, for increasing the quality of the rendering, and for displaying the box inside which the volume is defined.

**Note:** This feature is only available with an OpenGL graphics level of 2.1 or higher.

#### 12.4.4 Exporting Surfaces

PrimeX maps can be exported in CNS (formatted or unformatted) or CCP4 format. To do so, select the map in the Surface Table, then click Export to Map. A file selector opens, in which you can choose the format, navigate to the desired location, and save the file.

# Customizing Maestro

Many aspects of the Maestro interface can be customized from within Maestro. This chapter describes customizing the panel layout, menus, keyboard shortcuts, mouse actions, and profiles, all of which can be done from Maestro. It also describes the resource files used for customization, which you can change by editing. Customization of the toolbars is described in [Section 2.4 on page 18](#) and customization of color schemes is described in [Section 7.2.4 on page 138](#). Setting preferences is described in [Chapter 14](#), and other customization tasks that can be performed using scripts are described in [Chapter 15](#).

The customizations described in this chapter can be saved explicitly, so that they are preserved in subsequent Maestro sessions. Customizations are stored separately for each profile, in the subdirectory (folder) for the profile in your *user profiles directory*, which is:

**UNIX, Mac:**     `$HOME/.schrodinger/maestrovv/profiles`

**Windows:**     `%APPDATA%\Schrodinger\maestrovv\profiles`

Here, *vv* is the two-digit Maestro version number (99 for this release). For Windows, `%APPDATA%` is `C:\Users\username\AppData\Roaming` (the location of shared application data).

For Mac, `$HOME` is usually `/Users/username`, while on Linux it is usually `/home/username`. The subdirectory where the data is actually stored is referred to here as the *profile*.

Other changes can be preserved only by creating a startup script that issues the Maestro commands necessary to generate the desired changes when Maestro is launched. For more information on startup scripts, see [Section 15.4 on page 382](#).

## 13.1 Changing and Saving Panel Layout

Although effort has been made to optimize the default window positions and dimensions, you may want to change them. Resizing and repositioning windows is done in the normal way by dragging a corner, a side, or the title bar of the panel. Here, “windows” means panels, dialog boxes, and the main window. You can also close all panels (except the main window), reopen the panels you had open, raise all panels, and arrange the panels in a cascade, from upper right to lower left, by choosing the corresponding items from the Window menu.

You can save the size and location changes in a layout file, by choosing **Save Layout** from the **Window** menu in the main window. Maestro immediately saves your panel settings to the file named `layout.res` in your profile. If you want to return the panels to their default sizes and locations, delete the `layout.res` file. If you change the panel size and location during a session and want to revert to the last saved layout, choose **Restore Layout** from the **Window** menu. You can also raise one or all open panels from the **Window** menu.

If you start Maestro and display it to a monitor with a lower resolution, or if you have fewer screens, some windows might not open in your display area. To fix this problem, quit Maestro, edit the coordinates of these windows in the `layout.res` file, or delete this file to reset the locations, and restart Maestro.

When you upgrade to a new version of Maestro, the panel layouts you saved in a previous version are not accessible in the new version. The reason for this is that, in the new release, panels are often upgraded and their elements rearranged. Using an old panel layout may hide important features of the panel. Once you have installed the new version of Maestro, start the program, arrange the panels the way you want them, and save the panel layouts. Maestro will use the new panel layouts for all subsequent sessions.

## 13.2 Customizing the Menus and Keyboard Shortcuts

The Maestro menus provide access to all the features of Maestro, organized mainly by function. You might want to rearrange the menu items, or even remove or rename menus and menu items, to suit your own needs. Along with changing the menu items, you can also change the mnemonics for the menus and the keyboard shortcuts.

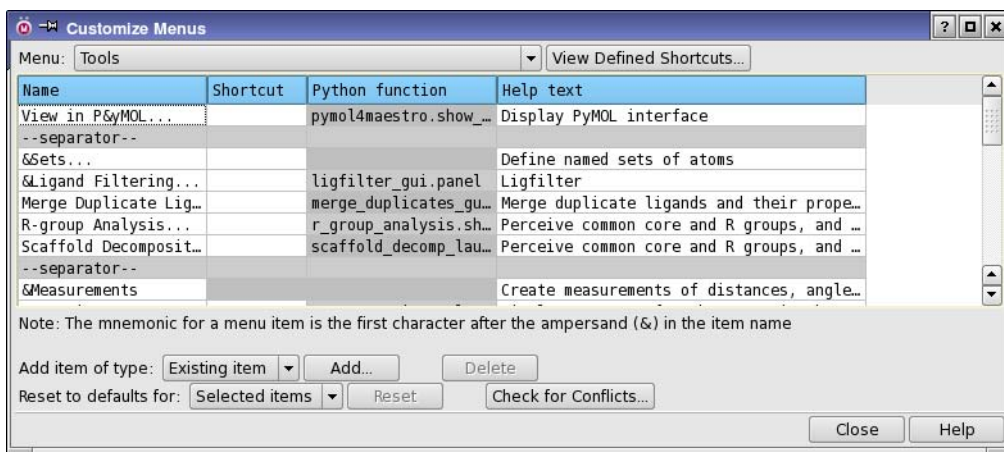


Figure 13.1. The Customize Menu panel.

The menus are defined in a resource file, which you can edit directly. This file is described in [Section 13.5.7 on page 325](#). However, you can easily customize the menus by using the Customize Menus panel, which you open from the Maestro menu in the main window for customizing main window menus, and from the Table menu in the Project Table panel, for customizing Project Table menus.

The Menu option menu lists all the available menus in the panel, including the menu bar itself. When you make a choice from this option menu, the items on the chosen menu are listed in the table. You can then make changes to the menu: change the name, the mnemonic, the shortcut key, and the help text; add and delete items, add separators and submenus. You can add the same menu item (function) to more than one menu.

**To change the item name and mnemonic:**

1. Click in the table cell to edit it.

The cell is outlined in blue to indicate that it is in edit mode.

2. Enter the new name and mnemonic.

The mnemonic is the letter that follows the ampersand (&) and is the keyboard key that can be used with the ALT key to open the menu or select the menu item.

**To add or to change a shortcut key:**

1. Click in the table cell to edit it.

The cell is outlined in blue to indicate that it is in edit mode.

2. Press the shortcut key that you want to use.

**To remove a shortcut key:**

1. Click in the table cell to edit it.

The cell is outlined in blue to indicate that it is in edit mode.

2. Right-click and choose Delete from the shortcut menu.

**To change the help text:**

1. Click in the table cell to edit it.

The cell is outlined in blue to indicate that it is in edit mode.

2. Type in the new text.

The help text is the text that is displayed in the Auto-Help bar at the bottom of the panel when you pause the pointer over the menu item.

**To move an item:**

1. Select the item.
2. Drag it to its new location.

**To delete menus or menu items:**

1. Select the table rows.
2. Click Delete.

**To add a menu item:**

1. Select the table row above which you want to add the menu item, or clear the table selection to add the item at the end of the list.
2. Choose an item type from the Add item of type option menu.
3. Click Add.

Subsequent steps depend on the item type:

- Existing item—the Add Existing Item dialog box opens.
  - a. Choose the item from the tree of the existing menus and items that are available in the current panel.
  - b. If you want to remove the item from its current location when it is added to the new location, select Remove from current location. Otherwise the item is duplicated in the new location.
  - c. Click OK.

The menu item is added to the menu with the existing name, mnemonic and shortcut.

- Python script—the Add Python Script dialog box opens.
  - a. Specify a name for the menu item in the Name text box
  - b. If you want to use a mnemonic, add an ampersand in the name before the mnemonic letter.
  - c. Specify the Python function that it runs.

The function is executed with the `pythonrun` command.
  - d. Click OK.
- Submenu—the Add Submenu dialog box opens.
  - a. Specify a name for the submenu in the Name text box



b. If you want to use a mnemonic, add an ampersand in the name before the mnemonic letter.

- Separator—a separator is added immediately.

If you want to revert any of your changes to the defaults, choose the scope of the reversion from the Reset to defaults for option menu, then click Reset. Choosing All menus resets all items to the defaults for the panel. Choosing Current menu resets all items for the current menu and its submenus. Choosing Selected items resets the name, mnemonic, shortcut, and help text only: it has no effect on any submenus.

To assist you in choosing shortcuts, you can view all the shortcuts defined in the panel by clicking View Defined Shortcuts. The Defined Shortcuts panel opens, showing a list of all menu items and their shortcuts. You can change the shortcut in this panel by editing the table cell and pressing the keys for the new shortcut.

When you have made changes, you can check whether the changes conflict with other menu items by clicking Check for Conflicts. This tool checks for conflicts and shows a panel that reports on the following items:

- Conflicts between mnemonics on the current menu.
- Missing mnemonics on any menu.
- A list of available mnemonic letters.
- Conflicts between shortcuts used for any menu item in the panel.

Not having a mnemonic is not strictly an error, but it means that you will not be able to choose the menu item from the keyboard.

## 13.3 Customizing Mouse Actions

If you want to change the Workspace actions that are associated with the mouse buttons or trackpad gestures, you can do so in the Customize Mouse Actions panel, which you open with Maestro → Customize → Mouse Actions.

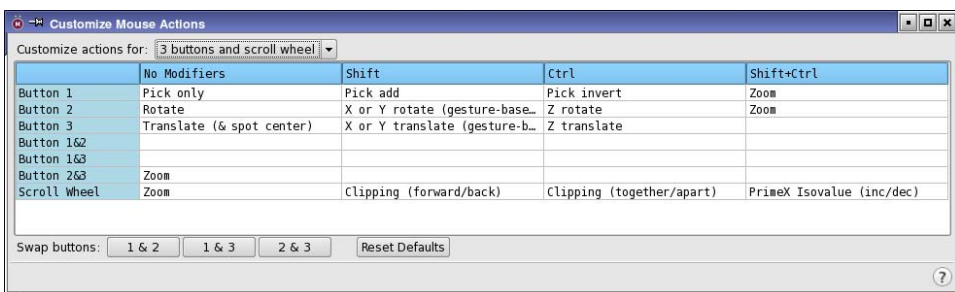


Figure 13.2. The Customize Mouse Actions panel.

First, choose the kind of device that you are using from the **Customize actions** for option menu. The choices include a mouse with 2 or 3 buttons, with or without a scroll wheel, or a trackpad. Button 1 is the left button, button 2 is the middle button (if present), button 3 is the right button. The table is filled in with the default actions assigned to each combination of modifier keys and mouse controls for the chosen device type. There is also a special PyMOL customization.

To change the action for a particular combination, click in a table cell. An option menu is displayed, from which you can select the action to use for that particular combination. Not all actions are available for each combination. You can assign the same action to multiple key/mouse combinations. The available actions are listed in [Table 13.1](#).

*Table 13.1. Actions that can be assigned to key/mouse combinations.*

<b>Action</b>	<b>Description</b>
No action	The mouse gesture is not assigned any Maestro action.
Rotate	Rotate around the axis that is perpendicular to the direction of movement of the pointer.
X or Y rotate (gesture-based)	Rotate around the <i>x</i> axis or the <i>y</i> axis, depending on the direction of the initial pointer movement (perpendicular to the rotation axis).
X rotate	Rotate around the <i>x</i> axis.
Y rotate	Rotate around the <i>y</i> axis.
Z rotate	Rotate around the <i>z</i> axis.
Translate (& spot center)	Translate in the <i>xy</i> plane in the direction of the pointer movement, spot-center with click (if relevant).
X or Y translate (gesture-based)	Translate in the <i>x</i> or the <i>y</i> direction, depending on the direction of the initial pointer movement.
X translate	Translate in the <i>x</i> direction.
Y translate	Translate in the <i>y</i> direction.
Z translate	Translate in the <i>z</i> direction
Zoom	Zoom in or out.
Clipping (forward/back)	Move the clipping planes forward (out of the screen) or back (into the screen).
Clipping (together/apart)	Move the clipping planes closer together or further apart.
PrimeX Isovalue (inc/dec)	Increase or decrease the Isovalue on PrimeX maps.

Table 13.1. Actions that can be assigned to key/mouse combinations.

Action	Description
Pick only	Pick atoms to create a new Workspace selection. Each pick clears the previous Workspace selection.
Pick add	Pick atoms to add to the Workspace selection. Does not affect other selected atoms.
Pick invert	Pick atoms to change their selection state. Does not affect other selected atoms.
Pick or Rotate	Pick atoms with click; rotate the Workspace with click and hold.
Rotate (Virtual Trackball)	Rotate around the $x$ or $y$ axis if the pointer is in a circle (virtual trackball) in the center of the Workspace, rotate around the $z$ axis if the pointer is outside this circle, with a smooth change in behavior over the boundary. The circle diameter is about 80% of the shortest Workspace dimension.
Pick or Rotate (Virtual Trackball)	Pick atoms with click; rotate the Workspace with click and hold using a virtual trackball (see previous item).

If you want to swap the actions in the table to use different mouse buttons, click one of the Swap buttons buttons. For example, clicking 1 & 2 would swap the assignments for Button 1 with those for Button 2, and swap the assignments for Button 1& 3 with those for Button 2& 3.

The default mouse actions are stored in the file `default.mouseactions` in the [Maestro resources directory](#). If you customize actions, the file is written to your profile.

## 13.4 Customizing Profiles

When you save any information that customizes Maestro, it is stored in your [user profiles directory](#) under the name of the profile you are using. This profile is in one way a custom profile, because it differs from the profile settings stored in the installation. If you want to customize Maestro in more than one way, you can create named custom profiles from one of the existing standard profiles. These profiles are also stored in your [user profiles directory](#), with the name that you give it.

You can create custom profiles in the Customize Profiles panel, which you open by choosing Maestro → Customize → Profiles. A custom profile can only be created from the current profile. To create the profile, click New, and enter a name in the dialog box that opens. The name is case-sensitive, and should not contain spaces. The new name is listed under Available Profiles. The files for the current profile are copied to the new profile. Custom profiles always have a “parent” profile, which is the standard profile from which they originated. Some customization (including display of online help) is dependent on the parent profile.

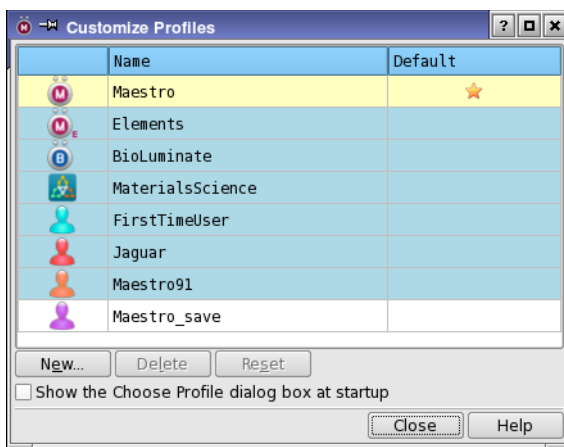


Figure 13.3. The Customize Profiles panel.

## 13.5 Customization by Editing Resource Files

Maestro uses resource and configuration files to make settings for various parts of its operation, for example, for the display of colors and fonts. The default versions of the resource files are stored in subdirectories of `$SCHRODINGER/maestro-vversion/data`. General resources are in the `res` subdirectory, which will be referred to as the *Maestro resources directory*. The default versions of project configuration files, rotamer resource files, and other resources are stored in `$SCHRODINGER/mmshare-vversion/data`, which will be referred to as the *installation resources directory*.

You can customize resources by copying the resource or configuration files to the relevant profile directory (folder) in your *user profiles directory*:

**UNIX, Mac:** `$HOME/.schrodinger/maestrovv/profiles`

**Windows:** `%APPDATA%\Schrodinger\maestrovv\profiles`

where `vv` is the 2-digit Maestro version, and then editing them. Instructions for editing these files are given in the subsections below.

When Maestro is started, resources and configurations are initialized from the Maestro resources directory, then resources that are set in the profile directory are read, and replace those read from the distribution. The resource files in the profile directory for a new release are copied from the profile directory for the previous release.

You can also change the standard resources and configurations by editing these files in the Maestro resources directory. If you do, the resources are changed for all users.

## 13.5.1 Visual Style Resources

To customize visual style resources, such as fonts and colors, you can copy the file `maestro.sty` from the Maestro resources directory into your profile directory as `maestro_user.sty`. The styles in the copy supersede the default styles, so you can remove lines from `maestro_user.sty` that you do not want to change from their defaults. This file is a QT style sheet, which is described in detail at <http://doc.qt.digia.com/4.4/stylesheet.html>.

The style sheet syntax has many similarities to the HTML cascading style sheets (CSS). To set the font used throughout Maestro to Arial normal 10px, for example, you would add the following lines to the style file:

```
*{
font-family: "Arial";
font-size: 10px;
font-weight: normal;
}
```

The font family, size, and weight for panel text can be set under General – Application fonts in the Preferences panel—see [Section 14.1.5 on page 334](#). For Workspace text, it can be set under Workspace – Fonts in the Preferences panel—see [Section 14.4.9 on page 348](#).

## 13.5.2 Color Definitions

Many of the places where color is used in Maestro use the RGB color values directly, rather than the Maestro color palette. The color palette is used for named colors. The default color palette is defined in the file `colors.res` in the installation resources directory (given above). When Maestro starts, it looks for a `colors.res` file in your profile directory and uses that copy in preference to the one from the installation resources subdirectory.

Maestro supports 256 colors in its color palette. Colors 1–128 are used by various parts of Maestro. Colors 129–256 are user-defined colors: these colors can be used for new color schemes and color ramps, for example. All of the colors are editable.

To customize the colors from Maestro, click the color button in the Bond Color tab of the Atom and Bond Coloring panel or in the Atom Labels tab of the Preferences panel. A color palette is displayed. Click Advanced, to open the Choose Color dialog box, then choose a color and click Edit to change the color. When you click OK, a `colors.res` file that contains the new color is written to your profile directory. To restore the default colors from the mmshare data subdirectory, click Restore Defaults in the Choose Color dialog box. This action removes the `colors.res` file from your profile directory.

You can edit the `colors.res` file directly with a text editor. Lines beginning with # are comment lines. Blank lines are ignored. Each line that defines a color has an index number, a

triplet of RGB color values in decimal format, and a color name. There must be no spaces after the name. If you change the resource file in the installation, the colors for all users are changed.

### 13.5.3 Color Schemes

Each of the standard color schemes is defined in a separate file in the `schemes` subdirectory of the Maestro resources directory. By convention, color scheme files end with `.sch`. The schemes are called by Maestro using the file `scheme.res`, which is in the Maestro resources directory. Color schemes can be created from Maestro—see [Section 7.2.4 on page 138](#) for details. Instructions for creating color schemes by editing the files are given below.

#### To define your own color schemes:

1. Create a `scheme.res` file in your profile directory, or copy `scheme.res` from the Maestro resources directory and edit it.
2. Create a `schemes` subdirectory in your profile directory.
3. Create color scheme files `scheme.sch` in the `schemes` subdirectory, or copy the `.sch` files from the `schemes` subdirectory of the Maestro resources subdirectory and edit them.

#### 13.5.3.1 The `scheme.res` File

The `scheme.res` file contains a three-line description of each scheme. The three lines contain the following information:

- The short name of the color scheme
- The long name of the color scheme. This is the name used in the Atom Coloring panel.
- The name of the file that contains the scheme definition

Lines beginning with a `#` are comment lines. Either the short name or the long name can be used to refer to the color scheme when using the `colorscheme scheme=scheme-name` command in Maestro.

#### 13.5.3.2 Color Scheme Files

The color scheme files contain a number of rules, one rule per line, which are applied in the order they appear in the file. Each rule consists of the name of a color as it appears in the `colors.res` file or the 6-digit hexadecimal code for the RGB color; an ASL specification that describes which atoms are to have that color; and an optional description. Color names must be a single token (there must be no spaces). If the color names do have an embedded space, they must be quoted (for example, "spring green").

The following is an example of a possible color scheme:

```
white atom.ele *
blue atom.ele N
red atom.ele O
```

This scheme first sets all atoms to white, then colors all the nitrogen atoms blue and the oxygen atoms red. Any number of such rules can be included in color scheme files.

### 13.5.4 Color Ramps

Color ramps are used in Maestro to map volume data onto a surface. In addition to the default color ramps provided with Maestro, you can also create your own color ramps. Like color schemes, each of the standard color ramps is defined in a separate file. These ramp files are stored in the `ramps` subdirectory of the Maestro resources subdirectory.

By convention, color ramp files end with `.rmp`. The color ramps are called by Maestro using the file `ramp.res`, which is stored in the Maestro resources subdirectory.

#### To define your own color ramps:

1. Create a `ramp.res` file in your [Maestro user resources directory](#), or copy `ramp.res` from the Maestro resources subdirectory and edit it.
2. Create a `ramps` subdirectory in your Maestro user resources directory.
3. Create color ramp files `ramp.sch` in the `ramps` subdirectory, or copy the `.sch` files from the `ramps` subdirectory of the Maestro resources subdirectory and edit them.

#### 13.5.4.1 The ramp.res File

The `ramp.res` file contains a three-line description of each ramp. The three lines contain the following information:

- The short name of the color ramp (used in Maestro commands)
- The long name of the color ramp (used in the Display Options dialog box of the Manage Surfaces panel)
- The name of the file that contains the ramp definition

Lines beginning with a `#` are comment lines. Only the short name can be used to refer to the color ramp when using the `surfacescheme colorramp=ramp-name` command in Maestro.

#### 13.5.4.2 Color Ramp Files

The color ramp files contain a list of color names, in the order that they will be used in the color ramp. The names of the colors must be taken from the `colors.res` file. Color names must be a single token (there must be no spaces). If the color names do have an embedded

space, they must be quoted (for example, "spring green"). Lines beginning with a # are comment lines. The following example defines a simple 5-color ramp:

```
# Number of colors
# 5
# Color names for all colors of this color ramp
red
orange
yellow
green
blue
```

When a color ramp is applied, the range of values that define the ramp is divided evenly between the colors. The first color on the list is applied to the most negative value, the last color to the most positive. If you want to extend the range of values mapped to a single color, you can duplicate the color in the list. For example, to extend the range for the endpoints in the above example, you could duplicate red and blue, as follows:

```
# Number of colors
# 7
# Color names for all colors of this color ramp
red
red
orange
yellow
green
blue
blue
```

### 13.5.5 Column Data in the Project Table

Several attributes of the property data and columns in the Project Table can be set in configuration files. The default precision to which real properties are displayed and the default units can be set in the file `m2io.ini`. The default initial column width in characters can be set in the file `mmproj.ini`; Boolean properties have a 2-character default width, and other properties have a 4-character default width. Since the column width and precision can be changed, these two values are only initial values. The two configuration files are stored in `$SCHRODINGER/mmshare-vversion/data`.

You can copy and edit these files to set the precision, units, and initial column width. The syntax for the files is given at the top of the file. You might want to set these values for properties that you use frequently and that are not generated from Schrödinger software. For example, you might want to specify the precision for properties read from an SD file; the name to use is `r_sd_SD-property`.



### 13.5.6 Property Families

When you create a custom property family (which you can do in the Manage Custom Property Families dialog box, see [Section 9.11.12 on page 239](#)), the definition is stored in your profile directory in the file `custom_property_groups`. Each custom family is defined on a single line as a comma-separated list, with the format

```
family-name, property1, property2, ...
```

Wildcard characters can be used to specify multiple properties.

Each built-in family has a set of default primary properties, which are essentially custom families, and are listed in the file `default.primary.properties` in the Maestro resources directory, with the same format as above. If you modify these primary properties, this file is copied to your profile directory as `custom.primary.properties` with the changes inserted. Primary properties are the properties that are shown by default in the Project Table. There is no interface for defining primary properties for custom families. To define primary properties for a custom property family, you can edit the `custom.primary.properties` file (or copy the `default.primary.properties` file to your profile directory and add the definition for the custom property family).

A given property can be present in multiple families. When the property is present, all families that contain the property are shown in lists of families: for example, many families include PDB ID as a property. To ensure that families are listed only if one of a set of key properties is present in the project, a key properties file can be defined, with the same format as for custom families. If one of the key properties are present, the family is considered to be present. If a family does not have key properties defined, the primary properties are used instead: if a primary property is present, the family is present. If primary properties are not defined, the family is present if one of its properties is present. The default key properties are stored in the `default.key.properties` file in the Maestro resources directory. There is no interface for setting key properties, so you must edit the file to change or add key properties, and write it as `custom.key.properties` to your profile directory.

### 13.5.7 Maestro Menus

The items that appear on menu bars and their menus are determined by the contents of a configuration file. The default configuration file is named `default.menu` and is stored in the Maestro resources directory. When you customize the menus from Maestro, the customizations are saved in the file `custom.menu` in your profile directory.

The menu file uses Json syntax to define the menu bars, the menus and submenus, and the items on the menus and submenus. Briefly, Json syntax defines objects using key-value pairs, in which the key is separated from the value by a colon, and pairs are separated by commas.

The key is a string, given in quotes. The value can be a string (in quotes), an object (in braces `{}`) or an array (in square brackets `[]`). Objects are lists of key-value pairs; arrays are lists of values.

Each menu bar, menu, or submenu is specified by a key-value pair in which the key is the unique identifier for the menu bar, menu, or submenu, and the value is an object. The object contains two key-value pairs:

- The `type` key defines the type of object, with the value `menubar` or `menu`. There is no distinction between a menu and a submenu: a submenu is just a menu that is on another menu rather than a menu bar.

The `deleted_standard_ids` type is used for a list of standard items that have been deleted from the menus. It is written when you customize the menus using the Customize Menus panel.

- The second key-value pair defines the contents of the menu or menu bar. If the object defines a menu bar, then the key is `menus`; if the object defines a menu, then the key is `items`. The value is an array that lists the menus or menu items (actions). For menus, separators can also be defined. Each element of the array is an object.

The menu and menu item objects have a number of keys that are common: `name`, `shortcut`, and `status_help`. The value for the `name` key is the name that is shown on the menu, and can include a mnemonic. It is required in all menu and menu item objects. In the example below for the Maestro main menu bar (truncated), the mnemonic is indicated by an ampersand preceding the mnemonic letter.

```
"main_window" : {
  "menus" : [
    {
      "id" : "main_maestro",
      "name" : "&Maestro",
      "shortcut" : ""
    },
    ...
    {
      "id" : "main_help",
      "name" : "&Help",
      "shortcut" : ""
    }
  ],
  "type" : "menubar"
},
```

The `shortcut` key value defines the key stroke for the item, and is usually only defined for menu items rather than menus. Shortcut keys are defined in the example below for the Maestro menu of the Maestro profile:

```

"main_maestro" : {
  "items" : [
    {
      "action" : "maestro_preferences",
      "name" : "Pre&ferences...",
      "shortcut" : "Ctrl+,"
    },
    ..
    {
      "name" : "separator"
    },
    {
      "action" : "maestro_quit",
      "name" : "&Quit...",
      "shortcut" : "Ctrl+Q"
    }
  ],
  "type" : "menu"
},

```

This example shows a separator item, which only has a name key whose value is separator. This item adds a horizontal line to the menu.

Menu objects have an `id` key that defines the unique identifier for the menu. Menu item objects have an `action` key that is also a unique identifier, for the action to be performed by the menu item. The action can refer to an standard Maestro action, or it can refer to a Python script. An example of both types of action is given below:

```

"Homology Modeling" : {
  "items" : [
    {
      "action" : "homology_model_simple_gui.panel",
      "name" : "Simple Homology Modeling...",
      "pyfunc" : "homology_model_simple_gui.panel",
      "shortcut" : ""
    },
    {
      "action" : "tasks_homology_modeling",
      "name" : "Advanced Homology Modeling...",
      "shortcut" : ""
    }
  ],
  "type" : "menu"
},

```

The first of these is a Python action, and the `action` key is the same as the `pyfunc` key. The `pyfunc` key defines the Python function that is executed to perform the action with the `pyfunc` Maestro command, in the form `module.function`. Python actions allow you to add your own Python scripts to the menus. Although, strictly speaking, you could define the

action key any way you like for a Python action, you should not modify the action key for any of the built-in Python scripts (other than defining aliases), as this key is used for other purposes in Maestro, to locate information on the action.

The second item in the example above is a standard Maestro action, i.e. one that is defined in the Maestro code. Standard Maestro actions have defined identifiers, which can represent opening a panel, or performing some operation in the Workspace, for example.

The definition of each standard Maestro action is required to be unique. If you want to use an action on more than one menu, you can use an alias for the action key, and point to the real action with the `std_action` key, as in the example below. This menu contains both menu items and a menu:

```
"QSAR" : {
  "items" : [
    {
      "action" : "phase_qsar_alias_1",
      "name" : "Atom-Based &QSAR...",
      "shortcut" : "",
      "std_action" : "phase_qsar"
    },
    {
      "action" : "phase_fieldqsar_alias_1",
      "name" : "Field-Based &QSAR...",
      "shortcut" : "",
      "std_action" : "phase_fieldqsar"
    },
    {
      "id" : "Property-Based",
      "name" : "&Property-Based...",
      "shortcut" : ""
    }
  ],
  "type" : "menu"
},
```

The action alias is formed by appending `_alias_n` to the standard action identifier, where `n` is an integer starting with 1. The action key must be unique, so the value of `n` should be incremented for each new alias. Aliases can also be used for Python actions, but the `std_action` key is not used because the action is performed using the `pyfunc` key value.

The name and `shortcut` keys for a standard Maestro action have default values, which are replaced if you specify them in the menu file. There are no defaults for Python actions.

Table 13.2 lists the available keys for a menu or menu item object.

Table 13.2. Keys used in specifying menus or menu items.

Key	Value
id	Menu or submenu. The value must be the unique identifier of a menu object.
action	Unique identifier of the action to be performed by Maestro when the menu item is chosen. It can be a standard Maestro action, or a name that you choose to be associated with a Python script, or it can be an alias. If it is an alias to a standard action, the <code>std_action</code> key must be given.
std_action	Unique identifier of a standard Maestro action, used when the action is an alias. Aliases are needed when the data associated with the action is modified for use in another menu.
name	Display name for the menu or menu item. The value is the name that appears on the menu bar or the menu. Append an ellipsis (three dots) to the name if the action is not completed by clicking on the menu item. Include an ampersand before the mnemonic letter, if needed. A special case of the value is <code>separator</code> , which includes a horizontal line on the menu.
pyfunc, pyfuncuser	Python function to be called when the action is performed, usually in the form <code>scriptname.method</code> . This key must be included if the <code>action</code> key for the menu item is not a standard Maestro action. Use <code>pyfunc</code> for Python scripts in the installation, and <code>pyfuncuser</code> for Python scripts installed in your user area.
shortcut	Shortcut key sequence for the action, such as <code>CTRL+O</code> .
type	Type of object. This key identifies whether the object is a menu or a menu bar. Allowed values are <code>menu</code> or <code>menubar</code> .

If you copy an action for a Python script to another location, you must change the `action` value by appending `_alias_n` to define an alias as well as changing the `name` value, if you want to use a different name.

The `pyfunc` key is intended for common scripts. When this key is used, Maestro searches for the Python module in the following locations:

- the directory specified by the environment variable `SCHRODINGER_SCRIPTS`,
- the common Python directory in the software installation, `$SCHRODINGER/mmshare-version/python/common`, for scripts available to all users.

The `pyfuncuser` key is intended for user scripts. When this key is used, Maestro searches for the Python module in the current directory or in the `scripts` subdirectory (folder) of your Maestro user resources directory.

If you delete standard Maestro actions from your menus in the Customize Menus panel, they are stored in a block with the type `deleted_standard_ids` (this is also the name of the

object). This block preserves the information on the deleted items, and makes it easy to restore them.

There are some items that cannot be configured by this mechanism. One of these is the Scripts menu, which is configured from the Manage Scripts panel. The others are the Quit item on the Maestro menu and the Undo item on the Edit menu. These items cannot be removed, and consequently the Maestro and Edit menus cannot be removed (though they can be renamed).

To make use of a customized menu that is not saved in your profile, you must start Maestro with the option `-u menu-file-name`. On Windows, you can add this option to your Maestro shortcut as follows:

1. Right-click on the shortcut and choose Properties.
2. In the Target text box, append `-u "path-to-menu-file"` to the text.

### 13.5.8 Rotamers

The rotamers that can be selected in the Rotamers dialog box are defined in a resource file, `rotamer.res`, which is stored in the installation resources directory. For each rotamer, the file lists the residue name, its frequency of occurrence (percentage), and the chi angles for the rotamer. You can copy this file to your Maestro user resources directory and edit it, if you want to make changes that apply to your own use of Maestro, or edit the copy in the installation resources directory if you want to change it for all users. If you want to add rotamers for a new residue type, check whether the residue type and its dihedrals are defined in the file `chidef.res`, and if not, add the appropriate definitions. This file is also in the installation resources directory.

# Setting Preferences

Maestro has an extensive set of options for the default settings in various panels and the default behavior of Maestro. These options can be set in the Preferences panel. To open the Preferences panel, choose Maestro → Preferences, or type CTRL+, in the main window. You can also open the Preferences panel with the relevant preferences displayed from the Project Table panel (Table → Preferences), the Manage Surfaces panel (click Preferences), and several other panels.

The preferences are collected into major groups, and in each of these there are collections of settings, or subgroups (described in the sections below). This classification is represented by a tree structure in the left of the panel, with turners to open and close the groups. Clicking on one of the “leaves” displays the collection of settings in the right of the panel, each of which contains controls for modifying Maestro’s default behavior. Some settings are in more than one collection, because they can be classified in several ways.

To find a preference, you can search for text that is in the tree text, the preference and heading text, or the preference tool tip text. Enter the desired text in the Search text box above the tree.

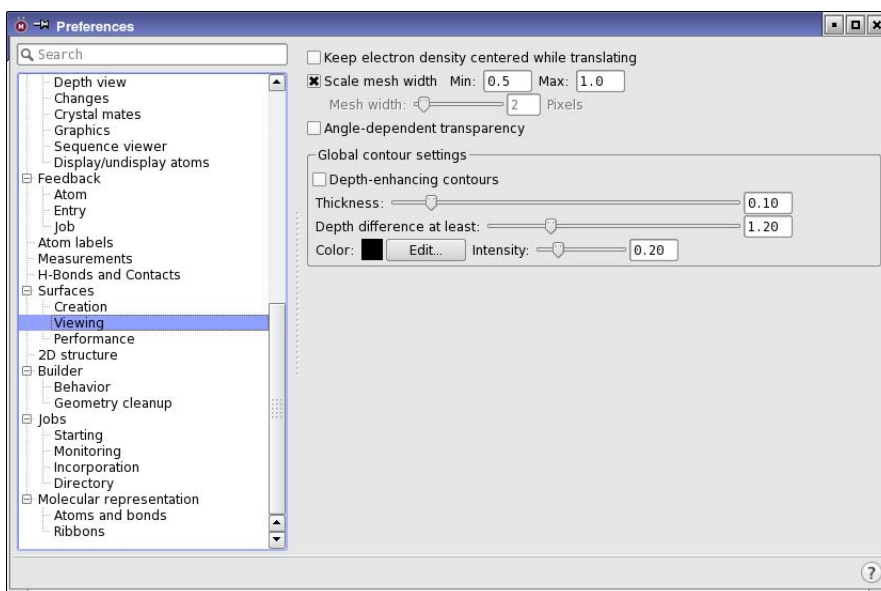


Figure 14.1. The Preferences panel.

As you type, the tree is pruned to show only the leaves in which the text is found. To show the full tree again, clear the text box by clicking the clear button at the right.

Changes made to settings in the Preferences panel are persistent: they define Maestro's default behavior until you modify them. A file called `prefer.cmd`, which contains all of your Maestro preferences, is created and saved to your profile. You should not edit this file directly, because Maestro overwrites it. If you want to add custom preferences that are not settable from Maestro, you should add them to a `maestro.cmd` file in your profile. This file is executed when Maestro starts, and takes precedence over `prefer.cmd`.

## 14.1 General Preferences

### 14.1.1 History

Command history

These options can be used to limit the number of Maestro commands stored, and therefore the number that is available in the Command Script Editor panel. Select **Unlimited** to keep all commands; select **Limited** and enter a value in the text box to limit the number of commands to the specified number.

Recently used project list

The most recently used projects are listed on the Project menu for quick opening. This text box allows you to specify how many projects are listed.

Log project operations to the annotations file

Keep a record of operations on the project in the project annotations file. The record of operations is displayed in the Project Summary panel.

### 14.1.2 Directories

The Maestro current working directory is the directory to which file, directory, and project selectors open by default, and to which job files are written. The default initial working directory on Linux is the Maestro startup directory, and on Windows and Mac is the Schrodinger folder in your Documents folder. By changing the settings in the Directory tab of the Preferences panel, you can specify a default current working directory.

You can choose from Maestro's current working directory, Project directory, Parent of project directory, Project jobs directory, and Other. These options are also in the Jobs–Directories section of the Preferences panel. See [Section 14.12.4 on page 370](#) for details of the options.



You can provide a custom directory that is linked to the Custom icon in the file, directory, and project selectors.



You can choose from two standard locations as well as your own location.

- **Maestro installation directory**—Set the custom directory to the directory in the installation that contains the Maestro software and resources. The actual path is displayed in the tool tip for this option.
- **Maestro launch directory**—Set the custom directory to the directory from which Maestro was started, on Linux, or the Schrodinger folder in your documents folder on Windows and Mac. The actual path is displayed in the tool tip for this option.
- **Other (specify below)**—Specify the directory in the Directory text box.

Maestro stores scratch projects in a temporary location, which you can specify in the Temporary project location text box, or click Browse and navigate to the desired location. The location should be large enough for your temporary projects, and for efficiency should be on a local file system. This location will be used for temporary projects the next time you start Maestro. You can also set the temporary location in the `SCHRODINGER_TEMP_PROJECT` environment variable. This value overrides the preference specified here.

In the absence of any specification, the `TMPDIR` environment variable is used for the location, followed by the default Schrödinger temporary directory, which is

**Linux, Mac:** `$HOME/.schrodinger/tmp`

**Windows:** `%LOCALAPPDATA%\Schrodinger\tmp`

On Windows, `LOCALAPPDATA` is set to `C:\Users\username\AppData\Local`.

See [Appendix A](#) of the *Installation Guide* for instructions on setting environment variables. If space is limited on `TMPDIR` or your home file system, you should consider setting the temporary location for projects.

### 14.1.3 File extensions

In this section you can change the default file extensions that are used when Maestro exports structures to a file. These extensions are appended to file names when you export structures from the Export dialog box if they do not already have an extension. They do not include extensions for file formats converted by Babel.

Extensions for compressed formats can be set for Maestro and SD files. On Unix, it can be useful to use the extensions `mae.gz` and `sd.gz`, so that the files can be recognized by applications such as `gunzip`. On Windows, use of `maegz` and `sdgz` ensures that the files can be associated with Maestro as the default application for opening them, whereas files ending in `.gz` are recognized as archives.

### 14.1.4 Appearance

#### Show tooltips

When the pointer is paused over a control, show information about the control in a box near the control after a short delay. The box is hidden after a period of time, or when the pointer is moved. This information in a box is known as a tool tip or balloon help.

#### Main title bar information

Show the selected information in the title bar of the main window, after the application name (Maestro). The version number is shown next to the application name, followed by the current working directory, if both are selected.

#### Set all toolbar styles to

Set the style for the toolbar buttons, by clicking the appropriate button. The style is applied immediately. The buttons can be displayed as icons, text, or both, with text beside or under the icon. Click the button for the style that you want to use. The Default button places text under icons for all toolbars except the Fragments toolbar (main window) and the ePlayer toolbar (Project Table panel).

### 14.1.5 Application Fonts

These font selection tools allow you to set the fonts for text in various parts of Maestro. You can choose the font type, the size, and the style. The text types you can set the font for are:

- Regular (text in all panels except for the items below)
- Text editing
- Project Table headers
- Project Table cells
- Toolbar buttons

An example of the font size is given below each set of font selection tools. You must restart Maestro to apply the new font size. The font size is stored in the file `maestro_user.sty` in your Maestro user resources directory (see [Section 13.5 on page 320](#)).

## 14.1.6 Panels

### Allow docking of panels

This option allows panels to be docked into the Workspace (main window) or into a “floating window” named Docked Panels, which is positioned to the right of the main window by default. You can choose where the panels are docked by selecting one of the Location options. Most of the panels other than those on the Applications and Workflows menu are dockable. This option is selected by default. If it is not selected, when you open these panels, they are opened outside the Workspace and cannot be attached to the Workspace (docked).

### Show dialog boxes at the position of the pointer

When a dialog box opens, center it on the current pointer position. If you turn this option off, the dialog box is displayed at its last displayed location (or its default location if it has not been displayed).

### Always show panels on top of main window

Show all panels in front of the main window, and ensure that they do not go behind the main window.

### Default homology modeling interface

Select the default interface to use for homology modeling, when choosing Tasks → Homology Modeling or Applications → Prime → Homology Modeling. The options are:

- Multiple Sequence Viewer—Use the Multiple Sequence Viewer panel for homology modeling.
- Structure Prediction Wizard—Use the Prime Structure Prediction panel for homology modeling.
- User choice—Open the Homology Modeling dialog box to present the choice between the two interfaces each time.

## 14.1.7 Quitting Maestro

Select the information that is shown or saved when Maestro quits.

### Warn when quitting Maestro

Display the Quit panel with controls described in this section when quitting Maestro. If the warning is not displayed, the actions selected by preferences in this section are performed without prompting.

### Warn if PyMOL is running when quitting

Display a warning if a PyMOL session launched from Maestro is still running when quitting Maestro. Quitting Maestro also forces termination of this PyMOL session, so the warning enables you to save any work done in PyMOL before Maestro quits and closes PyMOL.

### Save panel layout

Save the panel layout (size, location) of all panels that have been opened in a Maestro session in a resource file when Maestro quits. The layout is read the next time Maestro is started. You can also save the layout by choosing Window → Save Layout.

### Write command log file

Write a log of commands used in the Maestro session to the log file specified in the text box. The log file is written to Maestro's working directory.

## 14.2 Project Preferences

These preferences govern opening and closing of projects, properties, Project Table display, and saving modifications of a Workspace structure to the corresponding project entry.

### 14.2.1 Opening and Closing Projects

#### Open last project on startup

You can choose to open the last project you were working on when you start Maestro. This feature is particularly useful if you are working on one project over a period of time. You can always open a specific project when you start Maestro under UNIX by using the `-p` option. See [Section 2.1 on page 11](#) for more information on Maestro options.

#### Show Project Table

Display the Project Table when you open a named project. This is the default behavior, but it does not apply to the scratch project.

#### Show Entry List

Display the Entry List when you open a named project. This is the default behavior, but it does not apply to the scratch project.

#### Warn before closing a scratch project

When closing a scratch project, show the Save Scratch Project dialog box, which gives you the choice of saving the project with a name, discarding it, or canceling the operation that closes the project. This dialog box is shown if you explicitly close the project (Project → Close), open another project, or quit Maestro with a scratch project open.

#### Turn off Workspace Style Reapply when closing a project

When closing a project, turn off the Reapply button on the Style toolbar, so that the current style is not changed when the Workspace changes.

### 14.2.2 Backups

These settings can be used to make a daily automatic backup of the project that is open in your Maestro session, to control the number of backups (either automatic or manual), and to receive notification of the status of a backup.

For more information on project backups, see [Section 9.1.3 on page 175](#).

#### Automatic daily backup

Select this option to request an automatic daily backup of the current project. The following options can be set for the backup:

##### Schedule for

Schedule the backup for the specified hour (on a 24-hour clock).

##### Post-backup check

Choose an option for checking on the success of the backup. The options are:

- None—Do not do any checking.
- Project exists—Check that the backup project exists.
- Required files exist—Check for the existence of files inside the project that are required for a valid project.
- Count entries and properties—Check that the number of entries, number of included entries, number of properties, and other counts match.
- Entry structure files exist—Check that the structure files for each entry exist and are valid. This option unzips the project temporarily, so it requires as much disk space as the full project.

### Send EMail notifications

Select this option if you want e-mail notification with details of the backup. If you select this option, you must fill in the information in the following fields:

- **SMTP server**—Full name of the SMTP mail server used to send e-mail notification.
- **Port**—Port to use for the SMTP mail server.
- **Security**—Type of security to use for e-mail. Choose from None, STARTTLS, or SSL/TLS.
- **From**—Full e-mail address of the user account from which e-mail notification is sent.
- **Password**—If sending e-mail requires a password, specify it in this text box.
- **To**—Full e-mail address of the user account to which e-mail notification is sent.

### Limit the number of backups

Select this option to limit the number of backups.

### Save at most N backups

Specify the maximum number of backups to save. This option is only available if you choose to limit the number of backups. When the number of backups exceeds this limit, the oldest backup is removed. This means that you must have space for one more backup than the number set, as the new backup is written before the oldest backup is removed.

### Display dialog

Select an option for when to display a notification dialog box after a backup finishes. The choices are Never, Only when an error occurs, and Always.

### Alternate backup location

Specify an alternate location for backups, by clicking Browse and navigating to the desired location. The location is shown in the text box when you click Choose in the directory selector that opens. When you first set an alternate backup location, the Alternate backup location option under Store new backups in is automatically selected, so that the new backup location is used.

### Store new backups in

Specify where to store new backups. You can choose from Same directory as project (the default), or Alternate backup location, to use the location you specified.

### 14.2.3 Entry Changes

#### Save workspace changes

When you include an entry in the Workspace, you are working with a copy of the structures in that entry. By default, Maestro saves, or *synchronizes*, changes in the Workspace version of the structure to the entry with which it is associated when you make the changes. The other two preferences allow you to dictate what changes are saved to the project. If you select *When approved*, you are prompted to save Workspace changes when you attempt to exclude that entry from the Workspace. If you choose not to save, your changes are lost. If you select *Only when specifically requested*, Maestro does not prompt you to save changes made to Workspace structures: you must click the disk icon in the status bar to save any changes.

### 14.2.4 Importing Structures

#### Import associated data files

If the structure file has other data associated with it, the data can be imported into the project and associated with the relevant entries, by selecting this option. The mapping of the data to the entries is done in a file with the suffix `.smap`. This option is selected by default.

#### For Desmond files, import only first structure

If you want to import only the first structure from a Desmond CMS file, select this option.

#### For PDB files, read alternate locations

If the PDB file contains alternate positions, you can read them by selecting this option. If this option is not selected, the coordinates for the atoms with the highest occupancy are read, and the rest are ignored. You can display alternate positions from the Workspace menu.

#### Open Protein Preparation Wizard after importing PDB file

If you are importing a PDB file, you can select this option to open the Protein Preparation Wizard panel automatically when the structure is imported, so that you can prepare the protein for use in various applications.

#### For PDB files, color by conversion status

When importing a PDB file, color the structure by the status of the conversion. The color scheme is described in [Table 3.2 on page 50](#).

For pose viewer files, turn on pose viewing

If a pose viewer file is imported, you can perform the setup in the Project Table automatically by selecting this option. You can then immediately start viewing poses—see [Section 6.1](#) of the *Glide User Manual* for more information. This option is selected by default.

For SD files, create titles from

SD files often do not have a title property, so you must choose one to display in the project from the options under this heading. The default is SD molecule name. To specify an alternative property for the title, select SD property and enter the property name in the text box.

Replace Workspace

If this option is selected (the default setting), Maestro automatically clears existing structures from the Workspace. To import new structures without removing the Workspace contents, deselect this option.

Fit to Workspace following import

Structures that are imported are not necessarily centered on the coordinate origin, and might not be visible even though displayed. To ensure that the view is centered on the structures and zoomed to display all atoms upon import, select this option. (This setting is persistent between Maestro sessions.)

Include in Workspace

To specify which structures are to be included in the Workspace, choose one of the options from this option menu: No Imported Structures, First Imported Structure, or All Imported Structures. The default is First Imported Structure. If you choose No Imported Structures and Replace Workspace is selected, the Workspace is cleared.

Create groups for

Structures can be added to the Project Table as single entries or as groups. You can control how the entries are grouped on import by selecting an item from this option menu. By default, groups are created for files with multiple structures. The groups are named after the files, minus the extension. You can also create a single group for all structures from all imported files, and provide a name in the Group name text box.

Map SD properties to existing non-SD properties

Select this option if you want to map properties in an imported SD file to existing properties in the project other than SD properties. You can also choose whether to modify the mapping each time you import an SD file (Always) or not to use a mapping (Never). Choosing Never is the same as deselecting the main option. If you choose Always, to modify the mapping, the Map



Properties dialog box opens on import of an SD file. In this dialog box you can select a property from the project for each property in the input file (in the first structure). The property mapping is applied when the file is imported. The dialog box also allows you to save and load property mappings, so you can use different mappings for different files or projects.

## 14.3 Project Table Preferences

### 14.3.1 Properties

These options affect the display of properties and editing of properties.

#### Show Entry Name

This option controls whether the Entry Name property is shown in the table. It is hidden by default.

#### Show Stars in new projects

This option controls whether the Stars column is shown when a project is created. To control the visibility of this column thereafter, use the Properties menu of the Project Table panel.

#### Show 2D structure in new projects

This option controls whether the 2D structure is shown by default when you create a new project (including a scratch project). Thereafter, the visibility of the Stars column can be controlled from the Properties menu of the Project Table panel.

#### Warn when editing properties

When this option is selected, a warning dialog box is displayed when you edit a property value, and you must confirm the change to the property.

#### When new entries are added

These options control which new properties are shown in the Project Table when new entries are added.

- Show all properties—Show all new properties when entries are added.
- Show only primary properties—Of the new properties that are added to the Project Table, show only the primary properties. The exception is properties imported from an SD file, all of which are shown by default.
- Do not show any new properties—Hide properties that are not already displayed in the Project Table when entries are added. This option is useful if you have a particular set of

properties displayed that you are interested in and don't want the set to change when you add entries.

### Justification

These options determine how numeric and textual values are justified in the table cells. The options for each type of data are **Left**, **Center**, and **Right**. By default, numeric values are right-justified, which is equivalent to aligning numbers on the decimal point, because real properties are generally displayed with a fixed number of decimal places. Text is aligned left by default.

### Sort string values

These options affect the order in which sorting is done when the property used to sort the table is a string. This preference applies to other tables and lists in Maestro as well as the Project Table.

- **Alphanumerically**—Sort strings with upper-case letters before lower-case letters and lower-case letters before numbers. A sequence of digits is treated as a single number for the purpose of the sort. This allows a sequence of strings that have increasing values of the numerical part to be sorted in ascending numerical sequence, while the rest is treated as a string. For example, if the sequence of strings was `ligand $n$` , where  $n$  ran from 1 to 100, `ligand10` would follow `ligand9`, and `ligand100` would follow `ligand99`. In ordinary string sorting, `ligand10` would follow `ligand1`, and `ligand100` would follow `ligand10`.
- **Alphabetically**—Sort strings in case-insensitive alphabetic order, with numbers preceding letters (“dictionary order”). No special treatment is given to sequences of digits.

### Default precision for properties

Real-valued properties are displayed in the project table to a set number of decimal places (precision). Some properties have predefined precision. You can set the number of decimals used for properties that don't have a defined precision in this text box. This value is used as the default for new properties and properties that are imported and don't have a predefined precision. This setting affects only the display precision, not the value of the property itself.

You can set the number of decimal places for individual properties, and also choose to use E notation, in the Set Decimal Places dialog box—see [Section 9.11.7 on page 234](#).

### Show 2D image in Row column tooltip

When the pointer pauses in the Row column, show the structure as a 2D image in a tool tip.

Add *N* pixels of padding when fitting column width to data

Add padding of the specified number of pixels to either side of the column when using the commands that fit the columns to the data (Table → Columns → Fit to Data).

Scroll bar

The scroll bar in the Project Table can be placed on either side of the table. These two options allow you to choose which side to place it on.

### 14.3.2 Colors

These settings control the colors used in the Project Table. Each of the color settings show the color and have an Edit button to change the color. Some of the colors are optional, others are always applied. The optional colors are only applied in place of the default color.

Default

Set the color for unselected rows.

Selected entries

Set the color used for selected entries (rows), both inside and outside entry groups.

Partially selected groups

Set the color used for the group row when some but not all of its entries are selected.

Fully selected groups

Set the color used for the group row when all of its entries are selected.

Standard fixed area

Set the color used for the standard (default) columns in the fixed area. The color is only applied if this option is selected.

Nonstandard fixed area

Set the color used for the nonstandard columns in the fixed area (columns that you move to the fixed area). The color is only applied if this option is selected.

Row numbers

Set the color used for the row number column (Row). The color is only applied if this option is selected.

### Column headers

Set the color used for the column heading row (Row). The color is only applied if this option is selected.

### Highlight alternating rows

Select this option to use different shades of the colors for odd and even rows in the table.

### Show row borders

Draw a horizontal line at the bottom of each row to mark the boundary between rows.

### Reset to

These buttons reset the colors. Default sets the colors to the default values. Classic sets the colors to those used in Suite 2011 (Maestro 9.2) and earlier.

## 14.3.3 Groups

These settings control behavior related to entry groups.

### Warn when deleting entry groups

Post a warning dialog box when an empty group is about to be deleted. The default is not to post the warning.

## 14.4 Workspace Preferences

These preferences control the behavior of actions and appearance of objects in the Workspace.

### 14.4.1 Picking

These settings affect the appearance and behavior of picking actions in the Workspace (click or right-click).

#### Beep when picking

Select this option to make the system beep for each successful pick in the Workspace.

#### Picking cursor size

Choose a small, medium, or large picking cursor. The sizes are in pixels.

#### Show Workspace menu on right-click-and-hold

Select this option to display a shortcut (context-sensitive) menu when you right-click in the Workspace. You can set the time-delay for displaying this menu by entering a value in the Delay before showing menu text box. Right-clicking and dragging is used for translation of a structure. If the delay is too short, the menu might be displayed before you start dragging.

#### Ignore Workspace click when giving focus to main window

Ignore any click in the Workspace when the main window does not have focus, and you are clicking on it to give it focus. Setting this preference prevents an unintended action from taking place when you happen to click in the Workspace to get focus in the main window. This preference is on by default. If the focus policy of your window manager puts focus in the main window without clicking (follows mouse), you might want to turn this option off.

### 14.4.2 View Animation

#### Animate view changes

This option enables animation of changes in the view: the structure changes from one view to another over a period of time, rather than instantly. View animation is done when an automatic change in view is made, such as spot centering, resetting the view, and fitting to Workspace. The duration of the animation can be controlled by entering a value in the Duration text box.

Animation can be turned off if the distance over which the structure moves is greater than a given threshold, by selecting Limit animation distance, and entering the distance threshold in the Maximum distance text box. The default threshold is 10 Å.

By default, the animation has a constant speed (linear). If you select Non-linear animation, the animation starts slowly, speeds up in the middle, then slows down at the end. If you are using animation for a smooth change between multiple views, linear animation may be preferable.

### 14.4.3 Translation

#### Keep center of rotation fixed while translating

This option keeps the center of rotation at its current position in the Workspace when the structure is being translated. When the option is deselected, the center of rotation moves with the structure when it is translated. The default location for the center of rotation is the center of the Workspace. The center of rotation is updated by spot-centering and by a fit-to-Workspace.

Keep electron density centered while translating

When translating the Workspace structure, selecting this option ensures that the cube in which the electron density is displayed remains at the same place relative to the Workspace view. The effect is that the structure with its electron density appears to move through the cube. The size of the cube is set in the Manage Surfaces panel—see [page 307](#).

### 14.4.4 Rotation

Sensitivity in rotation

Use the slider to set mouse sensitivity for rotation. Larger values result in faster rotation.

Keep center of rotation fixed while translating

This option keeps the center of rotation at its current position in the Workspace when the structure is being translated. When the option is deselected, the center of rotation moves with the structure when it is translated. The default location for the center of rotation is the center of the Workspace. The center of rotation is updated by spot-centering and by a fit-to-Workspace.

Display center of rotation

Display a marker at the center of rotation. The marker is a set of three circles perpendicular to each other that indicate the orientation of the view.

Smoother local rotation

This option makes local rotation appear to happen smoothly. Turning it off can result in more jerky rotation, but may prevent rotation from continuing after the mouse has stopped moving.

### 14.4.5 Trackpad

The Trackpad section is only visible if you have a multi-touch trackpad.

Pinch gesture sensitivity for zoom

This slider controls the rate at which zooming is done as you pinch.

### 14.4.6 Transformations

Keep center of rotation fixed while translating

This option keeps the center of rotation at its current position in the Workspace when the structure is being translated. When the option is deselected, the center of rotation moves with the structure when it is translated. The default location for the center of rotation is the center of the Workspace. The center of rotation is updated by spot-centering and by a fit-to-Workspace.

#### Display center of rotation

Display a marker at the center of rotation. The marker is a set of three circles perpendicular to each other that indicate the orientation of the view.

#### Keep electron density centered while translating

When translating the Workspace structure, selecting this option ensures that the cube in which the electron density is displayed remains at the same place relative to the Workspace view. The effect is that the structure with its electron density appears to move through the cube. The size of the cube is set in the Manage Surfaces panel—see [page 307](#).

#### Include alternate positions in local transformations

When performing a local transformation on a set of atoms that include atoms with alternate positions, transform the coordinates for both alternatives. Deselect this option to transform the displayed location and not the alternate.

### 14.4.7 Dipole Moment

Choose options for the display of an arrow in the Workspace to represent the dipole moment.

- Show disk on positive end of arrow—Show a disk around the positive end of the arrow.
- Show positive and negative colors—Color the arrow with a color gradient from blue (negative) to red (positive).
- Show arrow from positive to negative—Show the arrow pointing from positive to negative (“chemists’ convention”). Deselect this option to show the arrow pointing from negative to positive (“physicists’ convention”).

### 14.4.8 Clipping Planes

These options affect the adjustment of the clipping planes (the planes between which objects are displayed, and outside of which objects are hidden).

#### Adjust clipping planes when focusing on a substructure

When zooming in to a set of atoms that has been selected by one of the processes listed below, adjust the clipping planes to within the distance specified in the Clip to within text box.

- Selecting a residue in the residues table of the Density Fit panel (PrimeX).
- Selecting a rotamer in the Residues table of the Rotamers dialog box.
- Middle-clicking a residue in the Workspace sequence viewer (to zoom in to it).
- Finding any set of atoms using the Find toolbar.
- Fitting a ligand to the Workspace.

### Zoom clipping planes with Workspace

Select this option to adjust the clipping at the same time as zooming in or out. The image in clipping planes window changes size when zooming, to reflect the new clipping planes settings. If this option is deselected, the clipping planes are not adjusted when zooming, and the image in the clipping planes window stays the same size. This option is off by default.

### Clip increment

Specify the increment by which the clipping planes are moved when you move them forward, backward, together, or apart (View → Move Clipping Planes). The increment is a percentage of the current width of the region between the clipping planes.

## 14.4.9 Fonts

These settings control the fonts used for text that is displayed in the Workspace: atom labels, measurements, adjustments, and single-entry feedback. It does not include caption or highlight text, for which there are separate font controls. You can choose the font type, the point size, and the style (bold or italic) using the option menus and buttons.

## 14.4.10 Fitting

### Fit to Workspace for these actions

These options control when an automatic fit to the Workspace is performed. The fitting only applies when you include entries in the Workspace: it does not apply to entry exclusion or to the results of job incorporation.

- Single entry inclusion—fit to the Workspace when the Workspace contents are replaced by the inclusion of a single entry from the Project Table or Entry List (Entry → Include or Entry → Include Only, click the In column).
- Stepping through entries (ePlayer)—fit to the Workspace when using the ePlayer or the left and right arrow keys to step through a set of entries, including only one entry per step. This does not include using the arrow keys to simultaneously include multiple entries.
- File import—fit to the Workspace when entries are added to or replace the Workspace when importing structures from a file.
- Other entry inclusions—fit to the Workspace when entries are included in other circumstances from the Project Table or Entry List. This option covers inclusion of multiple entries in the same operation.



#### Fit target

Select an option for the atoms that should be fitted to the Workspace when an automatic fit is done, from All atoms or Ligands. If you have multiple ligands, all ligands are included in the fitting procedure. The fitting itself is done to the displayed atoms of the selected target, and does not include undisplayed atoms.

#### Zoom clipping planes with Workspace

Select this option to adjust the clipping at the same time as zooming in or out. The image in clipping planes window changes size when zooming, to reflect the new clipping planes settings. If this option is deselected, the clipping planes are not adjusted when zooming, and the image in the clipping planes window stays the same size. This option is off by default.

#### Fit to Workspace when growing

When you are building a structure in Grow mode, Maestro fits the structure to the Workspace after each fragment addition by default. To prevent the fitting, deselect this option.

#### Enhance fog

Enhance the fogging depth cues when fitting to the Workspace.

#### Fit margin

Specify the margin in angstroms around the structures or selected atoms when fitting them to the Workspace.

### 14.4.11 Zooming

These settings affect the display when zooming in and out in the Workspace.

#### Zoom clipping planes with Workspace

Select this option to adjust the clipping at the same time as zooming in or out. The image in clipping planes window changes size when zooming, to reflect the new clipping planes settings. If this option is deselected, the clipping planes are not adjusted when zooming, and the image in the clipping planes window stays the same size. This option is off by default.

#### Minimum size of Workspace for automatic zooming

Set the minimum size of the Workspace in angstroms for automatic zooming, that is, zooming in that is performed as a result of other actions rather than user-initiated zooming. When this setting is on, zooming in stops when the distance across the Workspace either horizontally or vertically reaches the specified value. This option essentially imposes a maximum zoom level,

so that there is a limit to the displayed length of bonds, and a single atom will (in general) never fill the screen. It guarantees that a defined amount of context will always be visible in the Workspace when zooming in. The context is also affected by the Fit margin setting—see above.

### **14.4.12 Depth View**

These options control the enhancement of the depth view using approximate ambient occlusion, which takes into account the ambient lighting blocked by nearby atoms. It is applied only to atoms in the CPK representation.

Enhanced depth view

Turn on or off the enhancement of depth viewing. This can also be done from the View menu in the main window or by pressing D when the pointer is in the Workspace.

Depth factor

Use this slider to change the amount of depth enhancement applied.

Cutoff slider

Adjust the grid size for the ambient occlusion calculations. A larger grid includes more atoms, which is desirable when there are large pockets in a protein structure, for example. However, this also makes the calculation slower.

Restore Defaults

Restore the default values for the depth factor and cutoff.

### **14.4.13 Changes**

These settings control how changes in the Workspace are saved to the project.

- **Automatically**—Maestro automatically saves any changes to entries in the Workspace to the project.
- **When approved**—Maestro determines when changes will be lost if they are not saved, and prompts you to save the changes. You must make a choice before proceeding.
- **Only when specifically requested**—Maestro never determines that changes must be saved. You must explicitly synchronize changes or they will be lost. To synchronize changes, click the exclamation point in the status bar of the main window.

### 14.4.14 Periodicity

These settings control the display of markers for periodic structures in the Workspace.

#### Unit cell

Make settings for the display of the unit cell in the Workspace.

##### Show

Choose an option to display the unit cell boundaries, the lattice vectors, or both.

##### Line width

Adjust the width of the lines in the unit cell boundaries and the lattice vectors with this slider.

You can set the color of the lines using the color button, which opens a color selector.

#### Polyhedrons

Make settings for the display of polyhedrons

##### Polyhedron color

Set the color of the polyhedrons. Clicking the button opens a color selector. The current color is displayed on the button.

##### Opacity

Set the opacity of the polyhedrons.

### 14.4.15 Crystal Mates

#### Rename crystal mate chains

If you want to generate unique chain names for the crystal mates, select this option. By default the crystallographically related copies have the same chain name as the original.

### 14.4.16 Graphics

The setting in this section control features that relate to the graphics card or graphics libraries.

#### Requested OpenGL level

These options select the OpenGL library version that is used to draw objects in the Workspace. Two versions are available: 1.2 and 2.1. OpenGL 2.1 has features that are used to provide higher quality and improved performance of the rendering when using hardware graphics.

If you use `-SGL` when starting Maestro, the performance with OpenGL 2.1 is much slower than that of 1.2, because hardware acceleration is not being used. However, if you want a high-quality single image, for example, you can select 2.1.

The **Best** option selects the best available OpenGL level. OpenGL 2.1 is used if you have an NVIDIA or an ATI graphics card with proper driver support. OpenGL 1.2 is used if Maestro is started with the `-SGL` option, if Maestro is run over a network, or if OpenGL 2.1 is not available or is not adequately supported (as is the case for some graphics cards that claim OpenGL 2.1 support). The version actually used is displayed below the options.

### Full scene antialiasing

Turn on full-scene antialiasing, which smooths the appearance of objects in the Workspace.

### Quality

The settings in this section control the quality of the molecular representation. The settings depend on the OpenGL level set in **Workspace – Graphics** (see [Section 14.4.16 on page 351](#)). The OpenGL 2.1 implementation is usually much faster than the OpenGL 1.2 implementation, so settings for OpenGL 1.2 are not needed for OpenGL 2.1.

For OpenGL 1.2, the following settings can be made:

#### Use simplified representation when moving

When a structure is being moved in the Workspace, display it at lower resolution than when it is at rest, and in a simplified representation. This speeds up the operation on the structure. This option is off by default, but is turned on when you select the **Performance** rendering option on the **Style** toolbar.

#### Use thick lines for tubes when rotating

In the simplified representation, use thick lines (of the same thickness as the tubes) when rotating. This makes the simplified representation look a bit more like the normal representation. The default is to use wire frame representation for bonds in the simplified representation.

#### Moving resolution

Specify the resolution to use for the structure when it is moving, on a scale from 1 to 50. Lower numbers mean lower resolution (lower quality).

#### Resting resolution

Specify the resolution to use for the structure when it is at rest, on a scale from 1 to 50. Lower numbers mean lower resolution (lower quality).

For OpenGL 2.1, the following setting can be made:

#### Use faster sphere-drawing method

Use the faster method for drawing spheres. This method provides up to 20% speedup when there are many spheres in the Workspaces, such as for a protein in CPK representation. It is not used when perspective is enabled.

### 14.4.17 Sequence Viewer

These settings control how sequences are displayed in the sequence viewer. The options are also available on the Sequence viewer shortcut menu.

#### Wrap sequences

Wrap the sequence display so that long sequences are displayed across multiple lines with vertical scrolling rather than on a single line with horizontal scrolling.

#### Display SSA

Show the secondary structure assignment for the sequence.

#### Align by residue number

Align the sequences in the sequence viewer by residue number. (Does not affect the alignment of the structures.) This option enables gaps to be displayed in the sequence viewer.

#### Display non-protein molecules

Display non-protein molecules in the sequence viewer. Three lines are used, for ligands, waters, and ions.

#### Proximity cutoff

Set the distance cutoff for the sequence viewer proximity color scheme.

### 14.4.18 Display/Undisplay Atoms

#### Display Within includes nonpolar hydrogens

When displaying residues within a given distance of the currently displayed atoms, select this option to display nonpolar hydrogens. By default only polar hydrogens are displayed.

## 14.5 Feedback Preferences

### 14.5.1 Atom

These settings control the atom information that is shown in the status bar when you pause the pointer over an atom. By default, the changes you make apply only to the current project, and are stored with the project. You can also store the settings as preferences for all projects, by clicking Save Preferences.

Show atom feedback in Status Bar

This option enables the display of selected properties in the status bar when the pointer pauses over an atom in the Workspace. The last property in the list can be selected from the Property field list. The default for this property is the entry title. See [Section 2.5 on page 24](#) for more information about what is displayed.

Show index of object to pick

When picking in the Workspace, show the index of the object that is being picked (atom, molecule, ...) as the first item in the Status Bar, in the format `Pick: index`.

Show property

This noneditable text box shows the property that is displayed. To choose the property, click Select to open a property selector. This is the last property in the atom feedback. The default for this property is the entry title.

Save Preferences

Click this button to save the settings in this panel as preferences that apply to all projects. The default is that the settings apply only to the current project.

### 14.5.2 Entry

These settings control the information that is displayed in the Workspace for a target entry. By default, the changes you make apply only to the current project, and are stored with the project. You can also store the settings as preferences for all projects, by clicking Save Preferences.

Show single-entry feedback in Workspace

Display information about a single entry, termed the “target” entry, in the top left corner of the Workspace. The target entry is the entry defined by the following conditions:

- Only one entry is included in the Workspace
- More than one entry is included in the Workspace, but only one is not fixed
- More than one entry is included in the Workspace, but only one is selected

If none of these conditions is met, there is no target entry, and no feedback is displayed. The symbol in the In column of the Project Table is red for the target entry.

Include property names

Select this option to include the names of the properties in the single-entry feedback along with the property value, in the form *name : value*.

Show properties

List of properties to display in the Workspace for the target entry. You can select properties in the list to delete with the Delete button. To add properties to the list, click Add and select the properties in the property selector dialog box that opens. The default properties displayed are the entry title and the PDB ID.

Save Preferences

Click this button to save the settings in this panel as preferences that apply to all projects. The default is that the settings apply only to the current project.

### 14.5.3 Job

Show job status feedback in Workspace

Show the status of the last job submitted from the current project in the top left corner of the Workspace, in the format *jobname:status*.

## 14.6 Atom/Bond Labels Preferences

These preferences control the appearance and the location of atom labels. Changes made in the label preferences are immediately applied to existing labels.

Font

Choose the font type, size, and style for atom and bond labels and Phase feature labels.

Field separator

By default, the label fields are separated by a space. To add a separator such as a colon, semi-colon, or vertical bar, type the character in this text box.

### Display headings in labels

If you select this option, the label includes the descriptions of the label fields. For example, if you selected Molecule Number, the label is molnum=*n* instead of simply *n*, where *n* is the number of the molecule.

### Display one-letter residue names in labels

If you select this option, the one-letter residue names are displayed instead of the usual three-letter or four-letter names. Only the common (naturally occurring) residues have one-letter names; the rest are labeled “X”.

### Display H isotopes for element labels

When displaying element labels, use the isotope symbols for hydrogen (H, D, T). This option is on by default.

### X-offset and Y-offset

To reposition labels, enter new values in these text boxes. The offsets define the location of the lower left corner of the label relative to the atom position or bond midpoint.

### Show label when atom hides

Display labels for atoms that are hidden. Labels for hidden (undisplayed) atoms are shown in the Workspace, but do not appear to be associated with an atom. Undisplaying atoms is not the same as excluding entries from the Workspace. Labels, like ribbons, can only be shown for included atoms; however, these atoms need not be displayed.

### Color atom labels by

Select an option to control the color of the atom labels.

- Atom color—color the labels with the color of the labeled atom.
- Constant color—color all atom labels with the color shown. Click the color square to display a color palette, then select the color, or click *Advanced* to open the *Choose Color* dialog box in which you can choose from a wider range of colors.

### Color bond labels

Color bond labels with the color shown. Click the color square to display a color palette, then select the color, or click *Advanced* to open the *Choose Color* dialog box in which you can choose from a wider range of colors.



## 14.7 Measurements Preferences

The Measurements tab contains settings for the precision and appearance of measurement text in the Workspace.

### Display Precision

In this section you can set the number of places after the decimal point that are displayed for measurements. You can set the values for distances, angles, and dihedrals separately.

### Text

In this section you can make settings for the font and border for the display of measurements in the Workspace.

#### Font

Choose a font, a point size, and make the font bold or italic (or both).

Draw background-colored border around text

Select this option to draw a border around the measurement text in the background color. The default is to use a transparent background (no border).

#### Color

These settings control the color of the measurement markers. The color buttons open a color selector, which you can use to select a new color for the marker type.

#### Line Width

The Line width slider and text box allow you to set the width of the lines drawn to represent measurements, in pixels.

## 14.8 Non-Bonded Interactions Preferences

This group of settings controls the display of hydrogen bonds, halogen bonds, contacts, and pi interactions in the Workspace. See [Section 10.2.2 on page 249](#) for more information.

### 14.8.1 Criteria

These settings are used to set the criteria for defining hydrogen bonds, halogen bonds, and contacts.

### 14.8.1.1 H-Bonds

These settings control the cutoffs that define a hydrogen bond (H-bond). For display purposes, hydrogen bonds are defined by relations between four atoms: the donor hydrogen atom (H), the donor atom (D) bonded to H, the acceptor atom (A), and another neighbor atom (B) bonded to the acceptor atom A. The bond can be represented as D–H...A–B. The following relations must be satisfied for a valid hydrogen bond:

- The H...A distance must be less than a specified maximum distance.
- The D–H...A angle must be greater than a specified minimum value.
- The H...A–B angle must be greater than a specified minimum value.

Hydrogen bonds are not shown unless the structure has explicit hydrogen atoms.

The default values used by Glide and those used in Maestro are different.

#### Maximum distance

Specify the maximum distance from the H atom to the acceptor atom (H...A) for an H-bond to be identified. The Maestro default is 2.8 Å, the Glide default is 2.5 Å.

#### Donor minimum angle

Specify the minimum D–H...A angle for an H-bond to be identified. The Maestro default is 120°, the Glide default is 90°.

#### Acceptor minimum angle

Specify the minimum H...A–B angle for an H-bond to be identified. The Maestro default is 90°, the Glide default is 60°.

#### Set default criteria for

Click **Glide** or **Maestro** to set the defaults for the three criteria to those for **Glide** or **Maestro**.

### 14.8.1.2 Halogen bonds

These settings control the cutoffs that define a halogen bond. Halogens can act as donors or acceptors. As an acceptor it interacts with a hydrogen, so it is like a hydrogen bond but with its own characteristics. As a donor it interacts with an electronegative element in a similar way to hydrogen, but again with some differences.

Halogen bonds in which the halogen acts as donor are defined in a similar way to hydrogen bonds, by relations between four atoms: the donor halogen atom (X), the donor atom (D) bonded to it, the acceptor atom (A), and another neighbor atom (B) bonded to A, represented as D–X...A–B. The following must be true for a valid donor halogen bond:

- The X...A distance must be less than a specified maximum distance (2.8 Å, by default)
- The D–X...A angle must be greater than the minimum donor angle (120°, by default)
- The X...A–B angle must be greater than the minimum acceptor angle (90°, by default)

Halogen acceptor bonds likewise have relations between the donor H atom (H) and the atom bonded to it (D), the halogen acceptor (X) and the atom bonded to it (B), D-H...X-A. The following must be true for a valid acceptor halogen bond:

- The H...X distance must be less than a specified maximum distance
- The D–H...X angle must be greater than the minimum donor angle
- The H...X–A angle must be greater than the minimum acceptor angle
- The H...X–A angle must be less than the maximum acceptor angle

#### Maximum distance

Specify the maximum distance from the halogen atom to the other atom for a halogen bond to be identified. This value is independent of whether the halogen atom acts as an acceptor or a donor.

#### Donor minimum angle

Specify the minimum D–X...A angle or D–H...X angle for a halogen bond to be identified. This angle can be set independently for halogens as donors and halogens as acceptors.

#### Acceptor minimum angle

Specify the minimum X...A–B or H...X–A angle for a halogen bond to be identified. This angle can be set independently for halogens as donors and halogens as acceptors.

#### Acceptor maximum angle

Specify the maximum H...X–A angle for a halogen bond to be identified when the halogen acts as an acceptor.

### 14.8.1.3 Contacts

These settings define the distance ratios for contacts and allow the exclusion of certain types of contacts from consideration as contacts.

Contacts are classified into three types: good, bad, and ugly. The ranges for which contacts are so classified are defined by a ratio C, given by the following formula:

$$C = D_{12} / (R_1 + R_2)$$

where  $D_{12}$  is the distance between atoms 1 and 2, and  $R_1$  and  $R_2$  are the van der Waals radii of atoms 1 and 2. The contacts are classified into good, bad, and ugly based on this ratio. C must

be monotonically increasing for each of the contact types, that is  $C(\text{ugly}) < C(\text{bad}) < C(\text{good})$ . The default values are:

- Good:  $1.30 > C > 0.89$
- Bad:  $0.89 > C > 0.75$
- Ugly:  $C < 0.75$

Contacts essentially only consider the overlap of the outer parts of a charge distribution, and take no account of electrostatics. A “bad” contact could therefore be favorable if the atoms have the opposite partial charge. Some of these, such as H-bonds and 1,4 interactions, can be excluded from consideration as contacts.

### Cutoff ratios

These text boxes specify the cutoff ratios  $C$  for contacts to be considered Good, Bad, or Ugly. Distances for which the ratio is smaller than the cutoff (but larger than any cutoff that is smaller) are included in the contact category defined by that cutoff. Any distance ratio larger than the Good cutoff is not considered a contact.

### Exclude

These options control whether certain atom pairs are considered to be in contact or not.

- H-bonds—Do not consider the hydrogen and the acceptor atom in a hydrogen bond to be in contact. This option is on by default.
- 1,4 interactions—Do not consider pairs of atoms that are connected by a sequence of 3 bonds to be in contact. Intra-ring contacts are always excluded. This option is off by default.

## 14.8.2 Display

These settings control the color and line width of the nonbonded interaction markers, whether any interactions are displayed while adjusting or transforming structures, and if so, which interactions are displayed.

### Colors

The colors of the markers for nonbonded interactions can be changed by clicking on the color button and choosing a new color in the color selector that opens.

### Line width

This slider and text box allow you to set the width of the lines drawn to represent nonbonded interactions, in pixels.

Display interactions while adjusting or transforming structures

Select this option to display specified interactions while adjusting structures or transforming structures. The interactions are updated dynamically as you perform the adjustment or transformation. The interactions to display can be specified by selecting from the options given below this option.

## 14.9 Surfaces Preferences

The Surfaces section has three tabs, Creation, Viewing, and Performance. These tabs contain settings for the appearance and behavior of surfaces in the Workspace.

### 14.9.1 Creation

These options set the default appearance for new surfaces, which includes surfaces created directly in Maestro, and surfaces created on import of volume data into Maestro that have no information on appearance settings. These settings are the ones shown by default in the Surface Display Options dialog box.

Transparency

Set the default transparency of the front and back surfaces, and choose whether to link the two transparency values so that they are adjusted together.

Style

Set the default surface style: Solid, Mesh, or Dot. The default style is not applied to surfaces that have a predefined style (such as PrimeX and SiteMap).

Colors, by surface type

Set the default colors of surfaces, by the surface type. Paired surfaces are surfaces like molecular orbitals.

Darken colors by cavity depth

Darken the colors of molecular surfaces according to the distance from an iteratively smoothed, convex surface. The darkening enhances the depth perception of surface cavities. This preference applies to new surfaces. The effect can be controlled for individual surfaces from the Surface Display Options panel—see [Section 12.4.2 on page 308](#).

### Intensity

Specify the intensity of the darkening effect, on a scale from 0.0 to 1.0, where 1.0 applies the full effect, and 0.0 is equivalent to turning off the effect. Setting this value is useful when the cavities are deep.

Show surface manager when surfaces are created

Open the Manage Surfaces panel when surfaces are created.

### 14.9.2 Viewing

These options affect the appearance and behavior of all surfaces or surfaces of a particular type.

#### Keep electron density centered while translating

When translating the Workspace structure, selecting this option ensures that the cube in which the electron density is displayed remains at the same place relative to the Workspace view. The effect is that the structure with its electron density appears to move through the cube. The size of the cube is set in the Manage Surfaces panel—see [page 307](#).

#### Scale mesh width

When zooming in and out, selecting this option allows the width of the lines in the mesh representation to be scaled appropriately. The Min and Max text boxes provide the means to specify the minimum and maximum scaling factor that should be used for the mesh. The scaling factor is applied to the mesh width set with the Mesh width slider.

#### Mesh width (pixels)

Set the width in pixels of the lines in the mesh representation of the surface. Scaling of the mesh width is applied to this value.

#### Angle-dependent transparency

Vary the transparency across the surface, according to the angle the surface normal makes with the plane of the screen. The transparency is a minimum when the normal is perpendicular to the screen, and a maximum when it is parallel to the screen. Only available with OpenGL 2.1.

### Global contour settings

These settings are only available with an OpenGL graphics level of at least 2.1.

#### Depth-enhancing contours

Draw depth-enhancing contours on the edges of surfaces and when an edge is in front of another part of the surface by more than a defined distance.

#### Thickness

Set the thickness of the contour (in angstroms).

#### Depth difference at least

Set the minimum distance that an edge of the surface must be in front of other parts of the surface for the contour to be drawn.

#### Color

Set the color of the contour, by clicking the Edit button, and the intensity of the contour color, with the Intensity slider and text box. The intensity is the fraction of the contour color that is mixed with the surface color when drawing the contour.

## 14.9.3 Performance

### When rotating, draw solid surfaces as

These three options (Solid, Mesh, Dot) control how surfaces are drawn while they are being rotated. Choosing mesh or dot surfaces may result in quicker rotation.

### Use low quality transparency for surfaces

These three options (When rotating, Always, Never) allow you to choose when low-quality transparency is used for display of surfaces. Low-quality transparency speeds up the redisplay of surfaces after rotation, at the expense of surface display quality.

### Use random patterns for low quality transparency

These three options (When in interlaced stereo, Always, Never) allow you to choose when to use a random pattern for low-quality transparency. The regular pattern does not produce good results for interlaced stereo. This option is primarily intended for use with interlaced stereo to improve the appearance of transparent surfaces.

## 14.10 2D Structure Preferences

These preferences control the display of 2D structures in the Project Table and the 2D Viewer.

### Maximum number of atoms

To ensure that the displayed structure is not too small, a limit on the maximum number of atoms in any structure that is displayed can be set in the Maximum number of atoms text box. For entries that have more than this number of atoms, a message is displayed in the 2D Structure column about the size limit, instead of the structure.

### Maximum scale factor

The structure images that are generated are much larger than the table cells, and are scaled down to fit. Structures are scaled down by at least the amount specified in the Maximum scale factor text box, and may be scaled down further if they are large. Setting a small value of this factor ensures that small molecules are not displayed on a larger scale than large molecules: the benzene ring doesn't look bigger than the rings in a steroid, for example.

### Font size

This slider allows you to adjust the point size of the font that is used for text (such as atom symbols) in the generation of the original image (before it is scaled).

### Label margin

Scaling factor for distance between atom symbols and bond lines.

### Bond line width

Width of the bond lines in pixels, for image generation.

### Hash spacing

Width of the wedge bonds in pixels, for image generation.

### Bond spacing

Spacing between bond lines for multiple bonds in pixels, for image generation.

### Use color in 2D images

Color the atoms by element in the 2D images.



Show all hydrogens

Show all hydrogens, rather than leaving them implicit. Hydrogens on non-carbon atoms are always displayed.

Label all carbons

Display a C for each carbon atom, rather than leaving them implicit.

## 14.11 Builder Preferences

In the Builder tab you can set options to control the use of united atoms, automatic adjustment of bond lengths, removal of hydrogens to maintain valence during build operations, and deletion of terminal atoms. The options are persistent between Maestro sessions, and are selected by default.

### 14.11.1 Behavior

Allow united atom types while building

The use of united atom types can cause problems for users (especially Jaguar users) who do not want implicit hydrogen atoms in their structures. United atom types with implicit hydrogens are assigned by default when hydrogens are deleted from heavy atoms. If this option is deselected, united atom types are never assigned when atoms and bonds are explicitly deleted, atoms are retyped, or structures are drawn freehand. Instead, the atom types remain unchanged, or explicit radical types are assigned if they are available.

United atom types are used regardless of this option if a hydrogen treatment that requires united atom types is applied, or when reading in a structure file (such as a PDB file) that does not have explicit hydrogens present.

Adjust bond length when atom type is changed

When atom types are changed, bond lengths are automatically adjusted to give a “reasonable” bond length. This behavior is undesirable if the geometry is already correct (such as from a crystal structure) and it is only necessary to change the atom types. Deselecting this option prevents the adjustment of bond lengths.

Adjust number of hydrogens during build operations

The number of hydrogen atoms is adjusted by default to maintain a normal valence during formal charge, bond order, or retyping changes. This behavior is not always desirable, and can be prevented by deselecting this option.

### Delete terminal atoms

When you delete an atom, the terminal atoms that are attached to this atom can be deleted, or they can be left in place. Terminal atoms are atoms that are bonded only to that atom, such as hydrogen or a halogen. Deleting terminal atoms would not, for example, delete a methyl group attached to the deleted atom.

### Fit to Workspace when growing

When you are building a structure in Grow mode, Maestro fits the structure to the Workspace after each fragment addition by default. To prevent the fitting, deselect this option.

### Include alternate positions in local transformations

When performing a local transformation on a set of atoms that include atoms with alternate positions, transform the coordinates for both alternatives. Deselect this option to transform the displayed location and not the alternate.

### Include zero-order bonds when defining molecules

When determining which atoms are bonded together to form molecules, consider atoms that are joined by zero-order bonds to belong to the same molecule. This option is selected by default.

## 14.11.2 Geometry cleanup

These preferences specify how geometry cleanup is done. You can clean up the geometry by pressing U in the Workspace or by choosing Edit → Build → Clean Up Geometry.

### Geometry cleanup method

Specify the method used to clean up the geometry. There are two choices:

- **Built-in**—Use the built-in minimizer with the OPLS\_2005 force field. This method is faster and supports larger structures, but is limited to the elements supported by OPLS\_2005.
- **UFF**—Use the Universal Force Field with the associated minimizer. This method is slower, but covers a much wider range of elements. It supports up to about 5000 atoms.

This preference can also be set from the Clean Up button menu on the Build toolbar.

### Freeze unselected atoms during geometry cleanup

Select this option to freeze the atoms that are not selected during geometry cleanup with the built-in minimizer. By default, atoms within 5 Å of the selected atoms are restrained with a

moderate restraint, and atoms within 5 Å of these atoms are restrained with a much tighter restraint, while the rest of the atoms are frozen. This option does not affect cleanup with the UFF minimizer.

## 14.12 Job Preferences

These preferences specify the conditions under which jobs are monitored and are incorporated when they finish, whether the job name is kept, whether warnings about proteins are issued, and whether to keep job files from the wizard-like workflows.

### 14.12.1 Starting

#### Retain last job name used

When you start a job, the Start dialog box provides several tools for selecting a job name. If you want to retain the last name used (so that you can modify it for the next job, for example), select Retain last job name used.

#### Minimize disruption from jobs

The effect of job incorporation and monitoring on the Workspace and the Project table can also be controlled with the Minimize disruption from jobs option. When this option is selected, changes to the Workspace and the Project Table selection from job monitoring and incorporation are minimized. This means that the Workspace is only updated when an entry that is already in the Workspace is replaced in the Project Table, and the selection of entries in the Project Table is not changed. Structure monitoring is off, but monitoring and display of the Monitor panel are controlled by the preferences listed above.

For more information on job monitoring, see [Section 3.2](#) of the *Job Control Guide*.

#### Warn about use of unprepared proteins

If you start a job (such as a Glide grid generation) that uses a protein from the project, Maestro checks whether the protein has been prepared by the Protein Preparation Wizard. If it does not appear to have been prepared (as indicated by the prepared property), a dialog box is displayed in which you can mark the protein as prepared and continue, or cancel the job. Proteins that have been prepared earlier than Suite 2009 do not have this property by default, and so are treated as not prepared. To prevent the display of this dialog box, deselect the option Warn about use of unprepared proteins. Proteins will then be accepted regardless of their preparation, but will not be marked as prepared.

### Warn before overwriting existing job files

Display a warning dialog box when a job name is reused and job files will be overwritten if the job is run or the job files are written. If this option is off, no warning is displayed, and the files are overwritten. However, if the existing job is still running, the files will not be overwritten, regardless of this setting, and a warning is displayed.

### Allow use of web server for BLAST searches

Allow Prime to use the BLAST web site to perform a BLAST search. This option allows you to run Prime Structure Prediction without having a local copy of the BLAST database. If your query structures are proprietary, you should not select this option. (The option is stored in the file `web_blast` in your [user resources directory](#) as a single word, `allow` or `deny`.)

### Always run driver on remote host

When running jobs on a remote host, run the driver for that job on the remote host as well. This option is useful if you are running on the Cloud, as the driver must run on the remote host. Note that some jobs, such as Glide, Prime MM-GBSA, and Induced Fit Docking, rely on the driver running locally and using the local file system (`-LOCAL`) to ensure that jobs are restartable. Running these jobs on the remote host will prevent restarting.

### Enable job debug output (-DDBEUG)

When the job is run, print debugging output. This option is useful when running jobs for analysis by Schrödinger technical support. It is not stored between Maestro sessions.

## 14.12.2 Monitoring

### When starting jobs

Monitoring behavior when a job is started can be controlled with two options:

- **Start monitoring**—Start monitoring jobs when they are submitted. If this option is deselected, jobs will not be monitored, but they will be incorporated if your preference for incorporation does not include monitoring.
- **Open Monitor panel**—Open the Monitor panel when a job is started. This option applies only to jobs that are not started from wizard-like workflows, where the job status button can be used to open the Monitor panel. By default, the Monitor panel is not opened when a job is started.

#### Update Monitor panel every N seconds

Update the job status and related information for unfinished jobs that are listed in the Monitor panel at the specified frequency. If you have chosen to incorporate jobs automatically or when approved, jobs that are not being monitored may be incorporated during the status update, if their status changes to “completed”.

#### Show job status in Workspace status bar

Show the job status as a button on the right end of the Workspace status bar. The button shows the number of active jobs in the project and the total number of active jobs. The tool tip for the button gives information on various job categories, listing up to three in each category. Clicking the button opens the Monitor panel. The frequency with which this status is updated can be specified in the Update every *N* seconds text box.

### 14.12.3 Incorporation

These settings control what happens to jobs and files when the jobs finish. See [Section 2.9 of the \*Job Control Guide\*](#) for more information on job incorporation.

#### Incorporate completed jobs

Set options for the incorporation of jobs that have finished and are ready for incorporation:

- **Only when monitored**—Jobs are only incorporated when you monitor them in the Monitor panel.
- **When approved**—You are prompted to incorporate a job when it finishes and is ready for incorporation. If you choose not to incorporate, you must monitor the job to incorporate it. If you subsequently select another option, you must restart Maestro for the option to take effect on jobs that you chose not to incorporate.
- **Automatically**—Jobs that are ready for incorporation are incorporated automatically. Maestro is unavailable while the job incorporates. This is the default behavior.

A progress dialog box is displayed while jobs are incorporated, and you must wait until incorporation finishes before you can do anything in Maestro. Incorporation is only done for jobs from the current project. If you change projects, the option you select applies to the new project.

#### Keep workflow job files for

For the products that have wizard-like workflows, you can set options for the retention of job files. By default, these files are deleted on incorporation of the results.

The options for the three products are:

- CombiGlide—Keep job files for the Combinatorial Screening workflow.
- Phase—Keep job files for the Develop Common Pharmacophore Hypotheses workflow.
- Prime—Keep job files for the Structure Prediction workflow.

### 14.12.4 Directory

These settings affect the directories used when running jobs. The last two set job options: see [Section 2.3](#) of the *Job Control Guide* for more information on the options.

Default directory for job startup and file i/o

These settings determine the location that Maestro uses for creating job files and the location that Maestro initially uses for file input and output. This location is called Maestro's current working directory, also the job launch directory or the I/O directory.

When you choose one of the options below, the current working directory is set to the specified location, and the option you select is stored as a preference. The current working directory is then set to this location when you start Maestro again. In the descriptions below, the directory is called the *default* directory. For more information on changing the current working directory, see [Section 1.4](#) on page 7.

**Note:** If you choose a default directory that is inside the project, you should wait until any jobs launched from that project finish before you rename the project, or save the project if it is a scratch project (which renames it to a named project).

- Maestro's current working directory—Set the default directory to the Maestro [startup directory](#). Jobs running with this setting are not lost if the project is renamed.
- Parent of project directory—Set the default directory to the parent directory of the current project (the directory that the project is in). Opening a different project or closing a project (which opens a scratch project) changes this directory. For zipped projects, the parent directory is the directory that contains the `.prjzip` file, rather than the temporary directory into which the zipped project is extracted. Jobs running with this setting are not lost if the project is renamed.
- Project directory option—Set the default directory to the top-level directory of the current project. This is the `project-name.prj` directory. This directory changes when a new project is opened, and therefore the current working directory changes. Jobs running in this directory will fail if the project is renamed. This includes saving scratch projects.
- Project jobs directory—Set the default directory to the project's jobs subdirectory (`project-name.prj/jobs`). This directory changes when a new project is opened, and therefore the current working directory changes. Jobs running in this directory will fail if the project is renamed. This includes saving scratch projects.

- Other (specify below) option—Use the specified directory as the default directory. You must enter the desired directory name in the Directory text box.

Copy archived job directory to the launch directory when job finishes (-SAVE)

When a job finishes, create a zip file of the temporary directory that the job used to write files needed for the job (the *job* directory), and copy it back to the job launch directory. The zip file is not automatically unzipped. This option can be useful if you need to debug a job that fails, and keep the files, or to use the files for some other purpose. Normally, these files (“scratch files”) are deleted and the directory is removed when the job finishes.

This option sends the -SAVE option to Job Control. It is not saved across Maestro sessions, but it is initialized from the `SCHRODINGER_SAVE_JOBDIR` environment variable.

Run the job in the launch directory and keep all files (-LOCAL)

When a job is run, use the launch directory as the location to write temporary files needed for the job, and leave the files in place when the job finishes. If the job launches subjobs, the subjobs might not use this directory for their working directory: the behavior depends on the application. If the subjobs do not write to the launch directory, you can set the Copy archived job directory to the launch directory when job finishes option to copy back the subjob temporary directories. Note that in this case, the files that are local already are not archived in a zip file.

This option sends the -LOCAL option to Job Control. It is not saved across Maestro sessions.

## 14.13 Molecular Representation Preferences

These preferences affect how atoms, bonds, and ribbons are displayed in the Workspace,.

### 14.13.1 Atoms and Bonds

These options control the default representation of atoms and bonds. There are three sections, and two general options which are described first.

Default representation

This option menu allows you to set the default representation to one of the five representations: Wire, Thin tube, Tube, Ball & Stick, or CPK. Selecting one of these choices from the menu sets the representation used for new atoms that are built or imported. If you import a file in Maestro format and it includes graphical information, the representation saved in the file is used rather than the defaults.

### Default color scheme

This option menu allows you to set a default color scheme for atoms and bonds. For some color schemes (which usually include the word Custom), a color option menu is displayed below the schemes option menu, so that you can choose the custom color. This option menu has a list of allowed colors. For a description of the standard color schemes, see [Section 7.2.3 on page 135](#).

### Restore defaults

Restore the default values for the atom and bond representation. This button is below the settings for the different representations.

### Wire settings

#### Scale wire width

If you want the wire width to scale as you zoom in, select this option. You can adjust the minimum and maximum wire (line) width in the Min and Max text boxes. The values are given in pixels, and there are limits on how much you can change these values that are determined by the OpenGL implementation on your computer.

#### Wire width

This slider you to determine the width of wire (in pixels) in the Wire representation.

#### Style

These options control how color is applied to bonds.

- **Split**—The bonds are split, and each half is colored with the color of the nearest atom.
- **Blend**—The color is progressively changed along the bond from the color of one atom to the color of the other. Selecting Blend can improve graphics performance.

#### Show bond orders

These options control when bond orders are displayed. Multiple bonds are displayed as multiple lines, and zero-order bonds are displayed as dashed lines.

The Automatically option displays bond orders at high zoom, when the portion of the displayed structure that is visible in the Workspace is less than 30 Å across. If you zoom out, bond order display is turned off; if you zoom in again, bond order display is turned on again when the display meets the criterion given.

The threshold for the display of bond orders can be changed with the Maestro command `repall borderscale=value`.



### Smoothing

These options request smoothing of the lines or tubes that represent bonds. Smoothing wire bonds especially enhances the viewing of larger structures. When Show bond orders is on, those bonds that are drawn with widths greater than one are not smoothed.

### Tube/Stick/CPK settings

This section has settings for the display of bond orders and the sizes of the tubes and spheres used in these representations.

#### Show bond orders

These options control when bond orders are displayed. Multiple bonds are displayed as multiple tubes, and zero-order bonds are displayed as tube segments.

The Automatically option displays bond orders at high zoom, when the portion of the displayed structure that is visible in the Workspace is less than 30 Å across. If you zoom out, bond order display is turned off; if you zoom in again, bond order display is turned on again when the display meets the criterion given.

#### Thin tube radius

#### Tube radius

These sliders set the radius of the tubes in angstroms for the tube representations.

#### Ball percentage

This slider sets the percentage of the van der Waals radius of the atoms that is used to determine the size of the spheres in Ball & Stick representation.

#### Stick radius

This slider sets the radius of the sticks in angstroms in Ball & Stick representation.

#### CPK percentage

This slider sets the percentage of the van der Waals radius of each atom that is used to determine the size of the spheres.

### **14.13.2 Ribbons**

These settings control the defaults for display of ribbons. The style and the color scheme are set when you create the ribbons.

#### Quality

Set the quality of the ribbon rendering. These options control the smoothness of the ribbons.

#### Use simplified representation when moving

Use a lower-quality ribbon representation when translating, rotating, or zooming. You might want to set this option if moving structures is slow when ribbons are displayed.

#### Blend ribbon colors

Select this option to create a smooth color transition on the ribbons between residues.

#### Helix interior

Select an option for coloring the interior surface of helices (and ladders). The two options are to use gray for the inside (Gray) or to use the same color as the exterior (Same as exterior), as determined by the color scheme.

#### Ribbon width

Set the width of ribbons in angstroms.

#### Ribbon thickness

Set the thickness of ribbons in angstroms.

#### Strand width

Set the width of strands in angstroms.

#### Strand thickness

Set the thickness of strands in angstroms.

#### Thin tube width

Set the width of thin tubes in angstroms. These tubes are used in Cartoon and Thin Tube representation.

#### Thick tube width

Set the width of thick tubes in angstroms. These tubes are used in CA Trace Tube and Thick Tube representation.

#### Ladder width

Set the width of the rungs of the ladder for DNA and RNA. The sides of the ladder are controlled by the ribbon settings.

#### Atoms to hide when ribbons are created

Select an option from this menu to determine which of the atoms that are associated with the ribbons are displayed or hidden when a ribbon is created. This option only affects the initial visibility; the normal atom display controls can be used to change the visibility of these atoms. The options are:

- None—Do not hide any atoms (the default).
- All associated atoms—Hide all the atoms associated with the ribbons, so that only the ribbons are displayed.
- Associated backbone atoms—Hide the backbone atoms, and show the side chains.

These options do not affect atoms that are not associated with the ribbons, such as ligands, cofactors, and water molecules.

#### Restore defaults

Restore the default values for the ribbon representation.

## 14.14 SMARTS Generation Preferences

This group of settings controls the generation of SMARTS patterns from selected atoms. There is one set of options, for including notational elements in the SMARTS pattern. Examples of the notation with the option selected are given next to the label.

#### Charge

Include the formal charge on an atom in the SMARTS pattern.

#### Number of substituents

Include the number of substituents that are attached to each atom in the SMARTS pattern.



# Scripting in Maestro

Maestro provides several facilities for creating and using scripts. You can create Python scripts or generate macros with the Macros panel and install them on the Scripts menu. You can also create scripts and assign them to one of the 12 function keys on your keyboard.

## 15.1 The Scripts Menu

The Scripts menu in the main window is configurable and allows you to install, manage, and run Python scripts or named macros directly from Maestro. Scripts can be installed by individual users, using the Install Scripts panel, or they can be installed in the Schrödinger software installation or some other suitable public directory for use by all users. Once scripts are installed, they can be managed from the Manage Scripts panel. The software installation contains a number of scripts that are installed on the menu by default.

### 15.1.1 Installing Scripts and Macros

Scripts or macros for individual use must be installed explicitly. To do so, you can use the procedures described below. Scripts or macros that are intended for general use need only be copied to the appropriate directory, and automatically appear on the Scripts menu. Instructions are given below for installation of scripts for general use.

#### To install a Python script:

1. From the Scripts menu, choose Install.

The Install Scripts panel opens (see [Figure 15.1](#)).

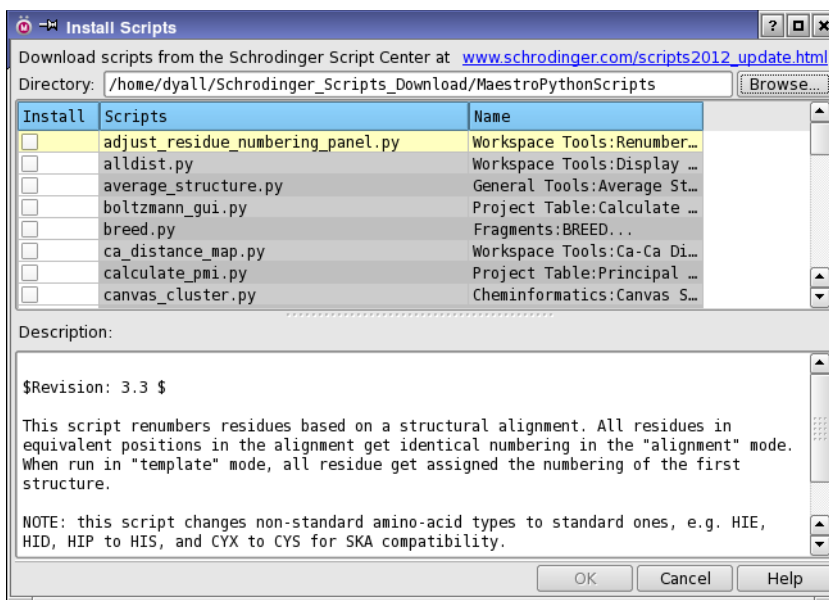
2. Enter a directory in the Directory text box, or click Browse and navigate to the directory that contains the scripts.

When the directory is entered, the table is populated with the available scripts.

**Note:** The Install Scripts panel only displays files with a `.py` suffix, the standard suffix for Python scripts, and only those files that are recognized as installable.

3. Click in the Install column to select a script.

The script name, the command that runs it, and a description (if available) appear in the text boxes at the bottom of the panel. The script name is what appears on the Scripts menu.



**Figure 15.1. The Install Scripts panel.**

4. Click OK.

The script is added to the Scripts menu and the panel closes. If the script is already on the menu, you are asked if you want to overwrite it.

#### To install a macro:

1. Choose Manage from the Scripts menu.

The Manage Scripts panel opens (see [Figure 15.2](#)).

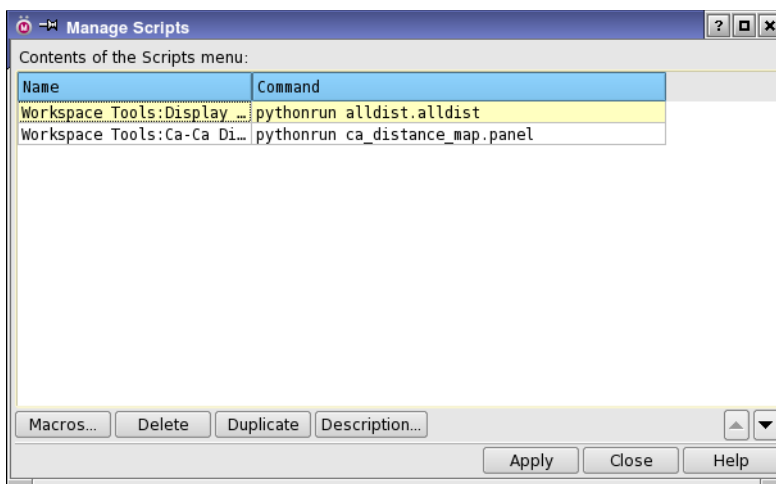
2. Click Macros.

The Macros panel opens. You can also open this panel by choosing Macros from the Edit menu.

3. Select a macro from the list.
4. Click Install.

#### To install scripts or macros for all users in the installation:

1. Copy the scripts to `$SCHRODINGER/mmshare-vversion/python/common` on Linux or Mac, or `%SCHRODINGER%\mmshare-vversion\python\common` on Windows.



**Figure 15.2. The Manage Scripts panel.**

2. Create or edit a `scripts.mnu` file in the same directory, and add the relevant lines to this file for each script.

**To install scripts or macros for all users in some other location:**

1. Copy the scripts to a directory that is accessible to all users.
2. Create or edit a `scripts.mnu` file in the same directory, and add the relevant lines to this file for each script.
3. Set the environment variable `SCHRODINGER_SCRIPTS` to the directory to which the scripts were copied. Make sure you use the full path.

The format for the lines in the `scripts.mnu` file can be deduced from the user installation. Briefly, each script should have a line containing the menu item, followed by a line containing the `pythonrun` or `macrorun` command to run the script.

### 15.1.2 Managing Scripts

The Manage Scripts panel provides some ways of managing the scripts that are installed.

To change the name or command of a script or macro, edit these fields directly in the Contents of the Scripts menu table.

You can delete or duplicate scripts and macros by using the Delete and Duplicate buttons. You can change the order in which the items appear in the Scripts menu by selecting a script and clicking the up and down arrow buttons.

To create submenus in the Scripts menu, edit the script names and insert a colon to separate the submenu name from the menu item. For example:

```
Color Atoms:Green
```

creates the submenu Color Atoms with the menu item Green.

To see the changes you have made to script names and locations, click Apply, then click on the Scripts menu. When you are satisfied with the changes, click Close to close the Manage Scripts panel.

To view the description of a script, first select the script in the table. If a description is available, the Description button becomes active. When you click this button, the description is displayed in a dialog box.

## 15.2 Using Python and Python Scripts

Python is a full-featured scripting language that has been embedded in Maestro to extend scripting facilities. The Python capabilities within Maestro include access to Maestro functionality for dealing with chemical structures, projects, and Maestro files, in an extensive API.

The two main Python commands used in Maestro are:

- `pythonrun`—executes a Python module. You can also use the alias `pyrun`. The syntax is:

```
pythonrun module.function
```

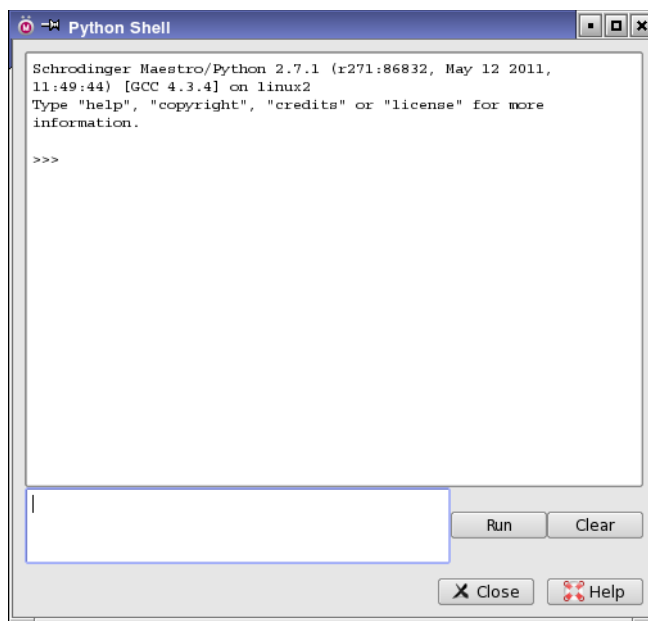
- `pythonimport`—rereads a Python file so that the next time you use the `pythonrun` command, it uses the updated version of the module. (You can also use the alias `pyimp`.)

The distribution includes a number of Python scripts designed for interaction with the structure in the Workspace. You can use these scripts, as well as create your own. You can also download scripts from the [Script Center](#). With the Maestro Scripts menu, you can install, manage, and run your Python scripts directly from Maestro. For more information on the Scripts menu, see [Section 15.1 on page 377](#).

Python commands can be run interactively in Maestro by using the Python Shell panel, which you open from the Window menu. This panel provides an input area where you can enter Python code, and then execute it. This input area has a range of modules preloaded, to make it easier to write code that interacts with Maestro:

```
from codeop import CommandCompiler, compile_command
from PyQt4 import QtCore, QtGui
from PyQt4.QtCore import Qt
```





**Figure 15.3. The Python Shell panel.**

```
import pythongui_ui
import sys, os, traceback, string
import pyhelp
from schrodinger.maestro import maestro
```

The command output is displayed in a text area in the panel. You can import other modules from the API for performing tasks in Maestro.

For detailed information on the API for using Maestro and other Schrödinger capabilities from Python, choose Help → Python Module Overview or Help → Python API Reference.

## 15.3 Scripting and KNIME Workflows

KNIME workflows are another way of scripting a sequence of applications that pass results from one application to the next. To create the workflows, you use the KNIME application—see the *KNIME Extensions User Manual* for details. KNIME provides the pipelining framework and a set of basic applications (“nodes”) that you can plug together to create a workflow. Schrödinger provides a set of KNIME nodes for its applications (the KNIME extensions).

Once you have created a workflow, you can generate a Python script to run the workflow. The script includes a panel so you can set up input values for the workflow, and manages the execution of KNIME in batch mode to run the workflow. These Python scripts can then be installed

on the Workflows menu so you can execute them in the much the same way as any built-in workflow. The panels to generate a Python script are also on this submenu.

You must purchase a license to run the Schrödinger KNIME extensions, except for the following:

- The reader and writer nodes (17 nodes)
- The file format converters (6 nodes)
- The Chemistry external tool nodes (5 nodes)
- The Python script nodes (6 nodes)

This means you can set up and run third-party applications from Maestro and make use of Maestro's features for processing the results without purchasing a KNIME extensions license. You can also use the KNIME-Maestro connector, the Run Maestro node, the Run Maestro Commands node, and the Run Canvas node without purchasing a KNIME extensions license.

For more information, see the *KNIME Extensions User Manual*.

## 15.4 Using Command Scripts

Some Maestro interface customization options can be set for the present session, but are not automatically retained for future sessions. To use these settings each time you launch a new Maestro session, you can create a startup script that will make the settings for you.

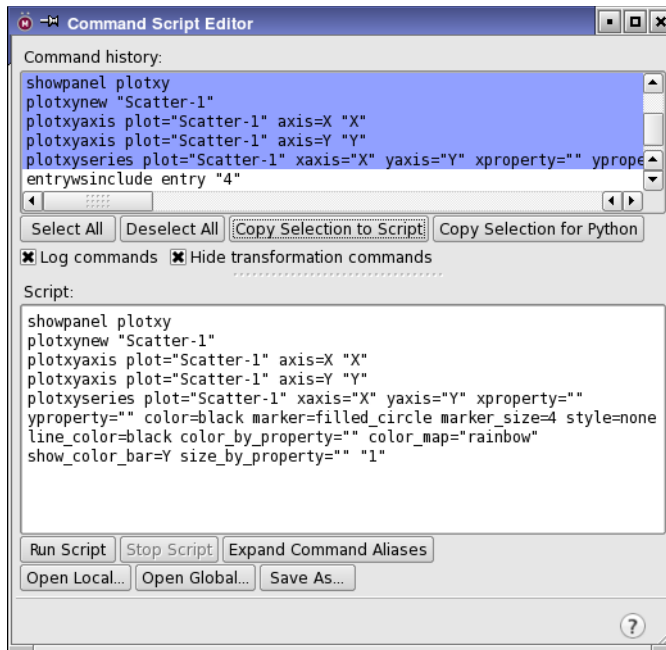
You can create startup scripts even if you are not familiar with the Maestro Command Language because most of the commands that you may want to include in a startup script can be extracted from the Command History log in the Command Script Editor panel.

To create a startup script, use the controls on the Command Script Editor panel, and then save the script in your preferences directory under the file name `maestro.cmd`. Each time you subsequently launch Maestro, this script is used to override the system-wide startup settings with your personal preferences.

To open the Command Script Editor panel, choose Window → Command Script Editor.

### 15.4.1 Command History

By default, most of the internal Maestro commands generated when you perform actions are logged in the Command History list in the Command Script Editor panel (see [Figure 15.4](#)). This written record of your commands is provided mainly to make the scripting process simpler. Since you can perform an operation, then cut and paste the resulting command into the Script list and save the script, it is not necessary to memorize the Maestro Command Language.



**Figure 15.4.** The Command Script Editor panel.

You can control whether Workspace transformation commands are displayed by using the Hide transformation commands option, and you can turn off command logging altogether by deselecting the Log commands option.

## 15.4.2 Building a Command Script

To build a command script from commands logged in the Command History list, you need to select and copy the commands of interest. Multiple commands can be selected with shift-click and control-click and by dragging. To select all of the commands in the list, click **Select All**. To deselect all the commands in the list, click **Deselect All**.

Once you have selected the desired commands, copy them to the Script text area by clicking **Copy Selection To Script**. If the copy operation takes more than a second or so, a progress dialog box is displayed. You can cancel the operation in this dialog box.

The commands are copied to the location of the cursor, which is placed at the end of the text after a copy operation. Therefore, repeated copy operations append the new command selection to the commands in the Script text area. If you want to create a new script, you must first delete the commands from the Script text area.

The commands in the Command History list remain selected after the copy operation, and must be explicitly deselected.

You can also directly enter commands in the Script text area.

### **15.4.3 Saving a Command Script**

To save the command script displayed in the Script text area, click **Save As** and navigate to the directory into which you want to place the file. Then type the name of the file to be created at the end of the line of text in the Selection box, and click **Write**. You must include the `.cmd` extension when specifying the file name.

Command scripts that call macros must not include the definition of the macro, or the script will not run properly. If you send someone such a script, you should also send the macro definitions.

### **15.4.4 Opening Existing Command Scripts**

The Command Script Editor panel provides two options for locating existing command scripts:

- Click **Open Local** to browse in your working directory.
- Click **Open Global** to browse in the `maestro-vversion/data/res` subdirectory of the Schrödinger software installation.

You can then navigate to the desired directory, select a command script, and click **Open** to load the script into the Script text area. If there are any commands currently in the Script text area, you are asked whether you want to replace them with the script you are about to open.

### **15.4.5 Running and Stopping Scripts**

After you load a script into the Script text area, you can execute it by clicking **Run Script**. If **Log commands** is selected, the script commands are added to the Command History list, even if the command script doesn't perform any operations that are visible in the Workspace.

If the script takes more than a second or so to run, a progress dialog box is displayed. You can stop the script in this dialog box.

### **15.4.6 Copying Commands as Python Commands**

If you want to use Maestro commands as part of a Python script, you can select the commands in the Command history list, then click **Copy Selection for Python**. Each command is wrapped as a Python command as

```
maestro.command('maestro-command')
```

and the commands are copied to the clipboard. You can then paste the commands into any application. For example, you can paste them into the Python Shell panel to create a Python script (see [Section 15.2 on page 380](#)). If you copy them to some other location, you must remember to import the Maestro Python modules in your script, otherwise they will not run.

## 15.4.7 Customizations You Can Perform With a Script

Some customization settings in Maestro are not persistent across sessions. You can configure Maestro on startup according to your personal preferences by performing any of the desired operations described below, making a script containing the resulting commands, and then saving the script as `maestro.cmd` in the preferences directory.

Before you create scripts to perform the following customizations, open the Command Script Editor panel, ensure that Log commands is selected and that all commands are shown.

If you already have a `maestro.cmd` file in your preferences directory and you want to save the commands in this file, open it in the Command Script Editor panel before you perform the new customizations. If you no longer want to override the system-wide settings with your personal startup preferences, delete your `maestro.cmd` file, or move it out of this directory.

After performing each customization, select the relevant commands in the Command Script Editor panel and copy the resulting commands into the Script text area. When you have completed all customizations, save the script.

### To set the Workspace background color:

1. Choose Workspace → Appearance in the main window.
2. Click the Background tab.
3. Click the Background Color button to choose a color in a color selector, or select one of the preset colors.

### To specify a stereo viewing method:

1. Choose View → 3D Options in the main window.
2. In the Stereo tab, choose a stereo display technique from the Method option menu.
3. Adjust the Size Factor and Scale Factor if necessary.

### To enable perspective:

1. Choose View → 3D Options in the main window.

2. In the Perspective tab, select Display in perspective.
3. Adjust the Perspective Scale, if needed.

**To hide the command input area:**

- Choose Window → Command Input Area in the main window.

Alternatively, you can type the following command into the Scripts text area, or add it directly to your `maestro.cmd` file.

```
hidepanel cominput
```

**To hide the clipping planes window:**

- Choose Window → Clipping Planes in the main window.

Alternatively, you can type the following command into the Scripts text area, or add it directly to your `maestro.cmd` file.

```
hidepanel topview
```

## 15.5 Creating Command Aliases

If you choose to use command scripts to perform operations in Maestro, you may find that there are many that you use frequently. The controls on the Command Alias panel allow you to assign shorter names to these commands. For example, you might want to define the alias label for the `labelatom` command. You can then use these aliases in commands typed in the command input area.

To open the Command Aliases panel, choose Maestro → Command Aliases.

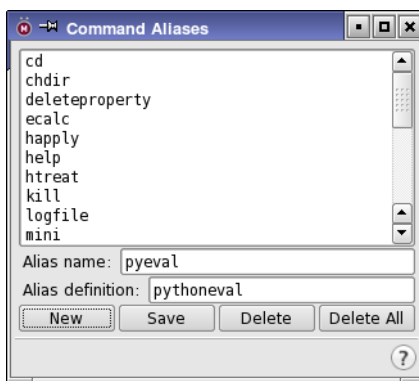


Figure 15.5. The Command Aliases panel.

### Defining a New Alias

To enter a new command alias, click **New**, type the abbreviation that you wish to use for the command in the Alias name dialog box, and click **OK**. In the Command Aliases panel, enter the command in the Alias definition box for the abbreviation you entered in the previous step.

### Saving Aliases

To save your aliases, click **Save**. The aliases are written to the file `alias.cmd` in your preferences directory. Once the aliases have been saved, they can be used in later Maestro sessions. If you wish to use an alias only for the current session, it is not necessary to save the alias.

### Changing an Existing Alias

Maestro is shipped with a set of command aliases already defined, and these can be edited or deleted. To change an alias, select the alias in the alias list, then type a new alias name or definition in the appropriate box.

To delete an alias from the list, select it and click **Delete**. To delete all currently defined aliases, click **Delete All**.

## 15.6 Creating Macros

Maestro allows you to create two kinds of macros: named macros and function key macros.

### 15.6.1 Named Macros

In the Macros panel, you can create a macro, name it, and run the macro from the command input area. To open the Macros panel, choose **Maestro → Macros**.



**Figure 15.6.** The Macros panel.

To create a named macro, click **New**, enter a name for the macro and click **OK**. In the **Definition** text box, you can either type the commands for the macro or copy and paste commands from the **Command Script Editor** panel. When you have finished entering commands, click **Update** to update the macro definition.

**Note:** Macros are automatically saved when you exit Maestro. However, it is advisable to update the macro whenever you change the definition. This makes the updated macro available during the Maestro session.

You can also add the macro to the **Scripts** menu by clicking **Add to Scripts Menu**. For more information on editing the **Scripts** menu, see [Section 15.1 on page 377](#).

To run the macro, enter the following in the command input area in the main window:

```
macrorun macro_name
```

If the command input area is not visible, choose **Window** → **Command Input Area**.

## 15.6.2 Function Key Macros

The **Function Key Macros** feature allows you to assign a script command, or series of commands, to a particular keyboard function key. You can use the keys **F2–F12**, on their own or with the **CTRL** key or **SHIFT** key or both. **F1** is reserved for the online help.

On Linux some of these keys are assigned by the window manager, and these assignments take precedence over user assignments. You can usually change or remove some or all of these assignments. If you are using the KDE window manager, go to **Control Center** → **Regional** → **Accessibility** → **Keyboard Shortcuts** → **Shortcut Schemes** → **Shortcut Sequences**. If you are using the Gnome window manager, go to **Preferences** → **Keyboard Shortcuts**.

To open the **Function Key Macros** panel, choose **Maestro** → **Function Key Macros**.

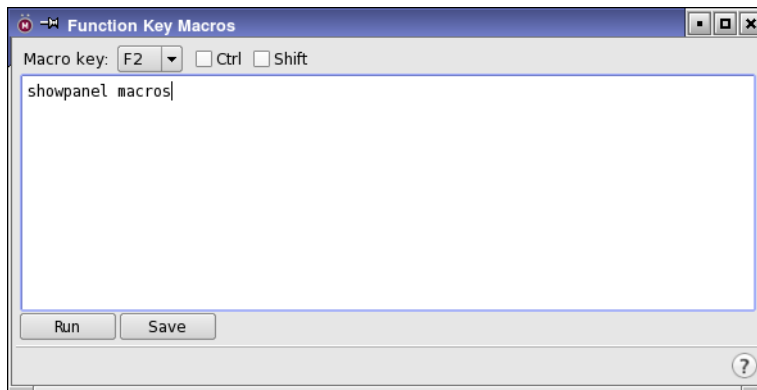


Figure 15.7. The **Function Key Macros** panel.



To assign a macro to a function key, choose the key from the Macro Key option menu, select the desired **Ctrl** or **Shift** options, and type the command or command sequence into the text area. You can copy and paste commands from the Command Script Editor panel into the text area of the Function Key Macros panel.

To test your macro, click **Run**.

To save a new macro for use in subsequent Maestro sessions, click **Save**. Saved macros are placed in the `maestro.mac` file in your preferences directory. To delete a macro, edit this file.



# Saving Workspace Images

In addition to creating structure files in a variety of formats, Maestro can produce images of the structures depicted in the Workspace. You can use the Save Image panel to create TIFF, JPEG, and PNG images, and you can copy images into other applications. For information on writing (exporting) structure files, see [Chapter 3](#).

## 16.1 Saving Images to a File

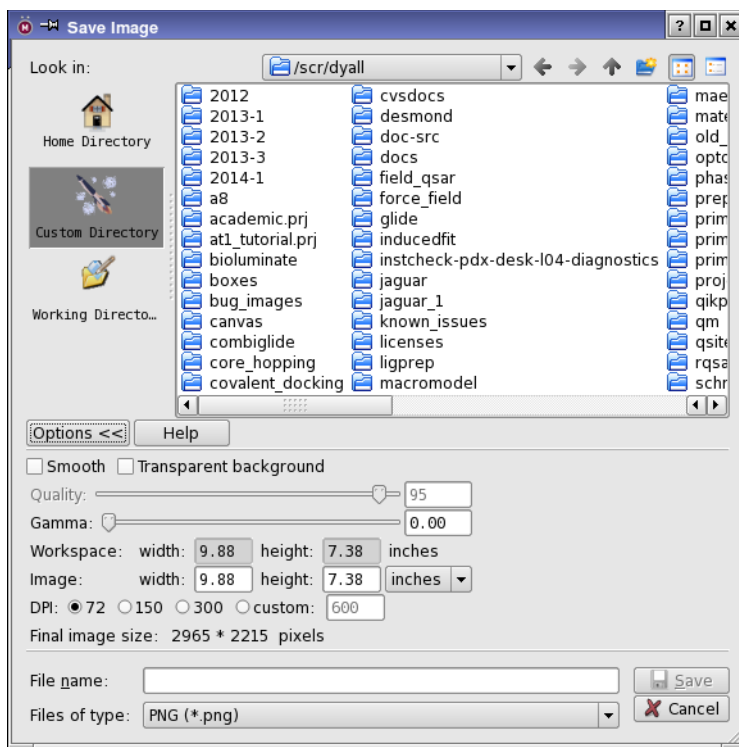
You can save images of structures rendered in the Workspace in TIFF, JPEG, or PNG format using the Save Image panel. To open the Save Image panel, choose *Workspace* → *Save Image*, or click the Save Image button on the Workspace toolbar.



The panel is a file selector that includes options for saving the image. These options are not displayed by default, but you can display them by clicking *Options*.

The Save Image panel allows you to set the following options:

- **Smooth**—Select this option to turn on scene anti-aliasing. This creates smoother edges, but takes longer to save the image.
- **Transparent background**—Save the image with a transparent background, instead of the Workspace background color.
- **Quality**—(for JPEG only) Use the slider to select a quality level from 1 to 100. The default is 5. The higher the quality level, the longer it takes to save the image. For high resolution images, this can take a while.
- **Gamma**—(for PNG only) Use the slider to select a gamma encoding level, from 0 to 1.
- **Workspace**—This noneditable area displays the dimensions of the Workspace in the units given for the image, below.
- **Image**—Enter the desired width and height of the image. These proportions are constrained, so if you change one parameter, the other adjusts automatically. To change the units, select either *Pixels* or *Inches* from the option menu.



**Figure 16.1. The Save Image panel.**

- **DPI**—Choose a resolution for the image or enter a specific value. If you choose Pixels for the units, this option is unavailable and the specified pixels are used.

The panel has two display areas that provide information about sizes:

- **Workspace**—Displays the measurement of the Workspace, not the whole main window. These values can not be edited directly. However, if you resize the Workspace, the values are updated automatically. The units are determined by the choice made for the image.
- **Final Image size**—Displays the final resolution of the image (in pixels). This value is not editable, but you can change it by changing the options above.

The image format can be selected from the Files of type option menu. The three supported formats are:

- **TIFF**—Images in TIFF format are saved without compression, and are “lossless” (all of the information in the original image is retained), but the file can be quite large. The TIFF format is recommended for saving high quality Maestro images.

- **JPEG**—JPEG is actually a compression method, not an image format. Maestro uses the JPEG-based JPEG-File Interchange Format (JFIF), the most commonly used JPEG file format. The JPEG file format specifies a means of compressing natural images that does not severely impair the perceived image “quality”. The JPEG method is almost always “lossy”, meaning that the reconstituted pixel data differs from that of the original. For natural images, these differences are not generally noticeable. However, in general, the JPEG method is not recommended for saving synthetic images like those Maestro produces, because there may be noticeable distortions in the saved image, such as subtle color changes. This option is provided because it allows you to create extremely compact screen shots for sending with an e-mail message or inserting in web pages.
- **PNG**—A bitmap image that uses lossless data compression. This format can also produce compact images. PNG stands for Portable Network Graphics.

When are you are ready to save an image, make sure the Workspace is unobstructed:

- Undisplay the clipping planes window by right-clicking it and choosing Hide or choose Window → Clipping Planes.
- Make sure there are no panels or dialog boxes overlapping the Workspace. This includes the Save Image panel.

**Note:** When saving high resolution images in wire molecular representation, you may need to adjust the wire width so that the bonds remain visible at the higher resolution. The automatic scaling of the wire width is used for larger images. The adjustment may take some experimentation, depending on the purpose of the image. See [Section 14.13.1 on page 371](#) for information on changing the molecular representation attributes.

**To save an image:**

1. Choose a format from the Files of type option menu.
2. If you want to increase the quality of a JPEG image, use the Quality slider to select the quality level.
3. Select the units you want to use: Pixels or Inches.
4. Adjust the image size (width and height).

The Workspace size can only be adjusted by actually resizing the main Maestro window.

5. Select a resolution under DPI. (If you chose Pixels above, this option is unavailable.)

The final image resolution is displayed in pixels near the bottom of the panel.

6. Navigate to a directory, and select or enter a file name.
7. Click Save.

## **16.2 Copying Images to Other Applications**

You can copy images of the Workspace to other applications using the clipboard. To make a copy of the image, choose Edit → Copy. The image is saved at the current screen resolution to the clipboard both as an image and as a pixmap. You can then paste the image into another application, such as a word-processing program.

---

# Using Maestro with Other Applications

As well as providing an interface to most of Schrödinger's software, Maestro also has interfaces to other applications. You can transfer data from Maestro to Canvas and to PyMOL, and you can copy structures between Maestro and applications like ChemDraw and Isis Draw. Maestro also has a plug-in that you can use with PowerPoint for visualization of structures. This chapter describes the ways in which Maestro can be used with these other applications.

## 17.1 Canvas

Canvas is Schrödinger's cheminformatics program. The Canvas GUI has its own projects and data storage that are separate from Maestro projects. You can export structures and data from the Project Table to Canvas. This feature is described in [Section 3.5 on page 60](#).

## 17.2 KNIME

KNIME is a program for graphically constructing workflows from various applications, which are encapsulated in "nodes" that can be connected, so that the output from one application is used as input to another. Schrödinger provides a wide range of KNIME nodes that can be used to construct workflows. KNIME workflows can be run from Maestro rather than from the KNIME interface or the command line, by wrapping a KNIME workflow in a Python script and installing it on the Workflows menu. The nodes that are used to communicate structures and data to KNIME do not require a license, so no specific license is required to run workflows containing only third-party nodes from Maestro.

In addition to running workflows from Maestro, you can send and receive structures to a running KNIME session from Maestro through a lightweight server that communicates with both applications. No license is required for this feature either.

For further information, see the *KNIME Extensions User Manual*.

## 17.3 PyMOL

For users who like to use PyMOL, Maestro provides a convenient way of transferring structures and associated data to PyMOL, via the PyMol for Maestro panel. This panel allows you to start PyMOL, load structures from Maestro to PyMOL, and make settings for the PyMOL

scene and image. You must purchase the “incentive” version of PyMOL to use this feature, because the components required for this feature to work are not in the free version.

To open the PyMol for Maestro panel, choose Tools → View in PyMOL in the main window.

Maestro uses the following sources to find an installation of PyMOL to use, in the order given:

1. On Windows, the registry.
2. The PYMOL4MAESTRO environment variable. This environment variable should point to the top directory of the PyMOL installation. This is the preferred method of specifying the location of PyMOL.
3. A PyMOL launch script called `pymol4maestro` in the Schrödinger software installation. This script must run PyMOL.
4. A PyMOL installation in `$SCHRODINGER/pymol`.
5. The standard PyMOL environment variable `PYMOL_PATH`.
6. On Windows, `C:\Program files\pymol\pymol`.
7. A launch script called `$SCHRODINGER/pymol`.

You can choose to send the Workspace structure or the selected entries to PyMOL. These structures are written to disk and then read by PyMOL, which is automatically started. You can also start PyMOL without sending structures to it by clicking Launch, and you can then hide or show the PyMOL panel by clicking the relevant button.

Once you have structures in PyMOL, you can use the PyMOL for Maestro panel to perform some of the PyMOL operations, like appending a scene to the list, stepping through scenes, updating and deleting scenes. You can choose whether to use ray tracing or rendering for the image, and save the current image, with the Image buttons. For the representation, you can use the closest match to Maestro’s representation with the Closest Match option, or use PyMOL’s representation by deselecting this option. You can also use the PyMOL or the Maestro mouse functions, with the Remap Mouse option, and show or hide the scene buttons in PyMOL with the Scene Buttons option. Finally, you can clear PyMOL, save a PyMOL session, and quit PyMOL with the PyMOL buttons.

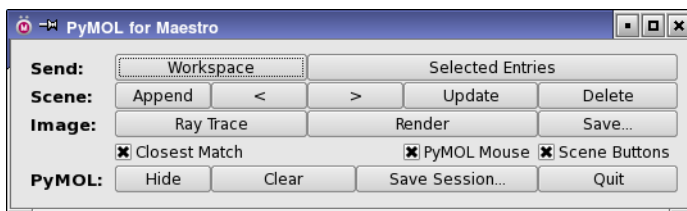


Figure 17.1. The PyMOL for Maestro dialog box.



If you are running Maestro and PyMOL on a Mac, you can use the X11 version of PyMOL rather than the native version, by selecting Use X11 in the PyMOL for Maestro panel.

## 17.4 ChemDraw and ISIS/Draw

When you copy a structure in ChemDraw or ISIS/Draw, it is placed on the clipboard as an object with an application-specific MIME type. Maestro recognizes objects with these MIME types, so you can paste them into the Workspace. The details of how the structure is pasted are given in [Section 3.7 on page 61](#). You must make sure that all atoms in the structure have explicit atom types, not generic metals (M) or organic groups (R).

In ISIS/Draw, you must set an option to enable copying to the clipboard in the appropriate MIME format. To do so, go to Options → Settings → General and select Copy Mol/Rxnfile to the Clipboard.

If you want to paste a structure from Maestro into ChemDraw, you can paste it as a SMILES string. When you copy a structure in Maestro, it is added to the clipboard as a SMILES string, which you can then paste into any other application that accepts a SMILES string.

## 17.5 PowerPoint

For PowerPoint presentations, Schrödinger provides a Maestro Viewer as an ActiveX control. This viewer allows you to take a copy of the data in the Maestro Workspace and display and manipulate the structure in the presentation, just as you would in Maestro. The data is stored in the PowerPoint document, so that it is always available in the presentation, and includes the atoms and their representations, ribbons, surfaces, measurements, labels, Workspace feedback, and Phase pharmacophore markers.

You must have the Visual C++ 2010 SP1 Redistributable Package and .NET 2 installed, both to create content for a presentation from Maestro and to use the ActiveX control in a presentation. These packages require administrator privilege to install. If .NET 2 is not installed, it is installed with the control; likewise the Visual C++ package is installed with Maestro. If the Visual C++ package and .NET 2 are already installed, you do not need administrator privilege to install the ActiveX control. More information is given in the Readme for the control.

To create the content for the presentation, you must have Maestro and the ActiveX control installed.

To view the presentation, you must have the ActiveX control and PowerPoint installed. You do not need a Schrödinger installation or a license to use the control for a presentation. The control can be used with PowerPoint 2003, 2007, and 2010.

You can download the Maestro Viewer control from the [Download Center](#), under Other Downloads.

The instructions below describe how to add the Maestro Viewer to a PowerPoint presentation. You must complete the installation as described above, then start PowerPoint. In PowerPoint, you must display the relevant tools, which you use to add the Maestro Viewer.

### **To add the Control Toolbox to the toolbar in PowerPoint 2003:**

1. Choose Tools → Customize.

The Customize dialog box opens.

2. In the Toolbars tab, select Control Toolbox.

The Control Toolbox opens.

3. Drag it to the toolbar.

The toolbox is now docked.

### **To add the Developer tab to the Ribbon in PowerPoint 2007:**

1. Choose Office Button → PowerPoint Options.

The PowerPoint Options dialog box opens.

2. Click Popular in the left panel.

The popular options are displayed in the right panel.

3. Select Show Developer tab in the Ribbon, and click OK.

The Developer tab is now added to the Ribbon.

### **To add the Developer tab to the Ribbon in PowerPoint 2010:**

1. In the File tab, click Options.

The PowerPoint Options dialog box opens.

2. Click Customize Ribbon in the left panel.

The ribbon customization options are displayed in the right panel.

3. Ensure that Main Tab is selected under Customize the Ribbon, on the right.

4. Select Developer in the tree, and click OK.

The Developer tab is now added to the Ribbon.

**To add a Maestro Viewer control to a slide:**

1. In the Control Toolbox (2003) or the Developer tab of the Ribbon (2007), click the More Controls button.



2. Select Schrodinger Maestro Viewer from the list of controls that is displayed.
3. Drag out a rectangle in the slide to insert the viewer.

**To add content from Maestro to the viewer control:**

1. In Maestro, set up the Workspace with the content that you want to use.
2. Press CTRL+C to copy the Workspace contents to the clipboard.
3. In PowerPoint, enter Slide Show mode (SHIFT+F5).
4. Click on the Maestro Viewer control.
5. Press CTRL+V to paste the Workspace contents into the viewer.

With the content in the viewer, you can rotate and translate the view in the same way as in Maestro. You can use the F3 key to make the molecule “rock”, or oscillate, around the y axis. You can use the wheel or the trackpad to zoom, provided the Maestro ActiveX control is active. To return to using the wheel for PowerPoint operations, ensure that the Maestro ActiveX control is not active.



# Help

This chapter describes the various ways in which you can obtain information on Schrödinger's products. Maestro has an online help facility, automatic context-sensitive help (Auto-Help), and tool tips (balloon help). Manuals in PDF format are included with the product distribution, and each product has a Known Issues page on the Schrödinger web site.

## 18.1 The Help Menu

The Help menu in the main window provides access to various kinds of information about Maestro and Schrödinger products. The items on this menu are described briefly below. Some of these items are described in more detail in later sections.

- **Help**—Opens the Help panel at the default help topic.
- **Manuals Index**—Opens the documentation index file in the Help panel. Click a link to view a manual or other document in your PDF viewer.
- **Search Manuals**—Opens the full text search index for the PDF documentation in Adobe Reader. You can then search across all the PDF documentation for words or phrases.
- **Python Module Overview**—Opens the top-level document that provides an overview of the Python modules supplied for use with Schrödinger software.
- **Python API Reference**—Opens the top-level document that provides access to detailed descriptions of the Python modules supplied for use with Schrödinger software.
- **Keyboard Shortcuts**—Displays a help topic that describes use of the keyboard keys in Maestro.
- **Tips**—Displays a help topic that provides tips for using Maestro.
- **Tutorials**—Opens the Tutorials panel, in which you can choose a tutorial, copy the files, and open the relevant manual.
- **New Features**—Displays a file that contains information on the new features in the current release.
- **Known Issues**—Submenu with a list of products for which known issues pages are available on the Schrödinger web site. When you choose a product from the submenu, the Known Issues page opens in your browser. If you are not logged on to the Schrödinger

web site, you are redirected to the logon page. After logging on, the page is displayed.

- Knowledge Base—Opens the Knowledge Base page on the Schrödinger web site in your browser.
- Diagnostics—Opens the Diagnostics panel, in which you can run licensing and installation diagnostic tests, and generate reports to send to technical support. See [Section 6.8](#) and [Section 7.6.1](#) of the *Installation Guide* for more information.
- About Maestro—Opens a window that gives information about Maestro versions and copyright and licensing notices.
- About Applications—Opens a help topic that gives a brief description of Schrödinger products.
- About Utilities—Opens your PDF viewer with the quick reference sheet that describes the utilities in `$(SCHRODINGER)/utilities`.
- Contact Technical Support—Displays a form on the Schrödinger web site that you can fill in to create a technical support ticket.

## 18.2 Maestro Help

For information on performing a particular operation in Maestro, look for answers first in the help. The help system includes descriptions of all the Maestro panels and how to use them, and other information on performing various tasks. In addition, it has active links to other sources of information, such as the PDF manuals and the Schrödinger web site.

The Maestro help is presented in the Help panel. You can open the help panel in the following ways:

- Click the Help button in the lower right corner of a panel or dialog box, or press F1. The button may have text or an icon.



A topic is displayed that gives information about the panel, dialog box, or current tab in the panel.

- Choose Help from the Help menu, or press CTRL+H (⌘H) in the Workspace. A topic is displayed that gives information about getting help.
- Choose Help from a shortcut menu in the Workspace, to open a relevant help topic.

Most topics contains a list of contents at the top that you can click to go to the relevant section, and a list of related topics at the end that you can click to select a new topic.

The Help panel has a toolbar at the top, with navigation and search tools. The Previous and Next buttons take you to the previous and the next topic or set of search results.



The Home button displays a list of all help topics with links, in alphabetical order.



To search for text across all topics, enter the words in the search text box, and press ENTER or click the Search button.



The results are displayed in the display area, and you can click the links to display the topic that contains the words.

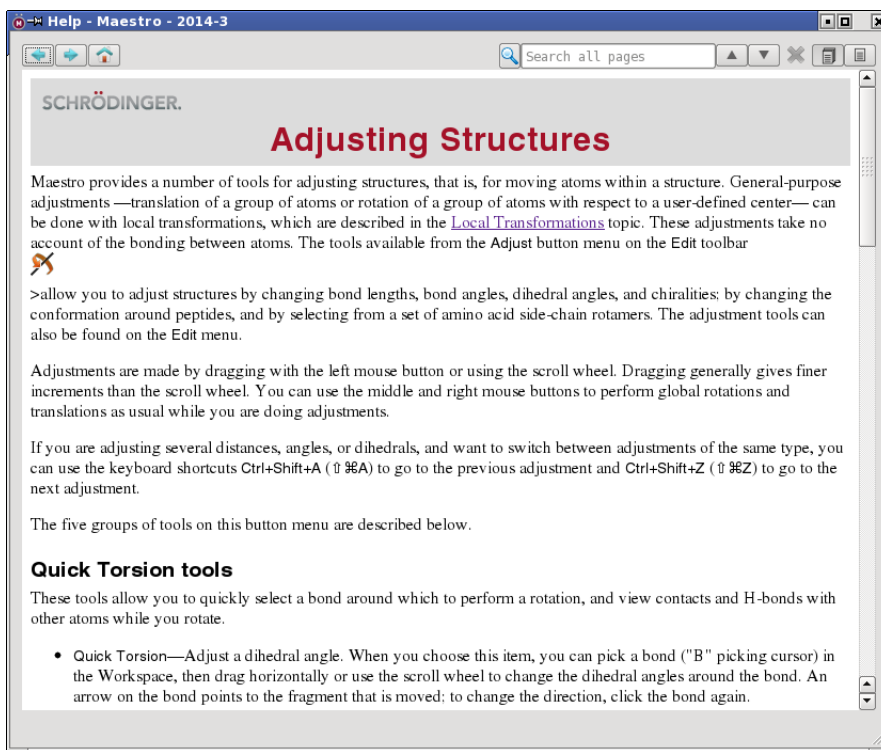


Figure 18.1. The Help panel.

By default, the search looks for all the words you enter (implicitly inserting “and” between the words). The search allows you to construct complex search expressions:

- Use ‘and’, ‘or’, and ‘not’ to construct conditional expressions. For example, ‘ligand preparation not protein’ finds topics that contain ‘ligand’ and ‘preparation’ but not ‘protein’.
- Use parentheses to group expressions, e.g. ‘(ligand not protein) preparation’ first looks for topics that contain ‘ligand’ but not ‘protein’, and then looks in the results of that search for topics that contain ‘preparation’.
- Use double quotes to search for an exact phrase, e.g. “protein preparation”.

To find words in a single topic, click the Find on page button.



You can then enter the words in the search text box and press ENTER or click the Search button. Click the arrow buttons to go to the next or the previous hit in the page.



### 18.3 Context-Sensitive Help

Maestro has two other help features, which are described below.

#### Auto-Help

The Auto-Help text area is located at the foot of the main window. The Auto-Help facility provides automatic context-sensitive help, usually providing information about the task to be completed. For example, when you open the Atom Labels panel, Auto-Help prompts you to pick an atom to label. Auto-Help is not available for all operations.

#### Tooltips

Tool tips (Balloon Help) consist of a floating text box containing context-sensitive help that appears when the pointer rests on an object. The box disappears when you move the pointer. You can temporarily disable tool tips by deselecting Show tooltips in the Appearance tab of the Preferences panel. Tool tips are available for many but not all interface components.



## 18.4 Manuals

Manuals are available in PDF format on the program DVD or the download, and are installed into the `docs` folder (directory) of your software installation. Manuals can be opened via the HTML documentation index `Documentation_Index.html` (Help → Manuals Index), or via a PDF index, `Manuals_Index.pdf`, which you can open in your PDF viewer. On Windows you can open the documentation index from the Start menu.

Manuals (and the PDF index) contain links to other manuals. As not all PDF viewers treat cross-document links correctly, we recommend the following viewers:

- Linux: `okular` or `evince`
- Mac: Adobe Reader
- Windows: Adobe Reader.

If you have Adobe Reader installed, in a version no earlier than 6.0, you can use the search index provided with the documentation to search the entire manual set. You do not need to load this index to search the documentation, but it makes the search much quicker. To make use of this index, choose Help → Search Manuals or open `Manuals_Search.pdx` in Adobe Reader, and then do the search. This file is stored in the `docs` folder. The problem with Adobe Reader on Linux does not affect the links to documents in the search results.

If you use more than one search index in Adobe Reader, you can select the Schrödinger index by following the instructions below.

1. Click Search.
2. Click Advanced Search Options at the bottom of the panel.
3. Under Look In, choose Select Index.
4. Navigate to and select the file `schrodinger.pdx`, which is in `$(SCHRODINGER)/docs`.
5. Ensure that this is the only index selected for searching.

If a document does not open when you click the link to it, the problem could be one of those listed below.

1. The document is not installed.

The installed documents are located in `$(SCHRODINGER)/docs/product`, where *product* is `maestro`, for example. By default, all the documentation is installed. See the [Installation Guide](#) for installation information.

2. The document was copied by the application and the relative links between PDF files are not preserved.

This can happen if the PDF reader is not used as a plugin in recent browsers. In some older browsers relative links are not preserved when a PDF file is opened with a plugin. One solution is to upgrade your browser. Another solution is to open this file directly in your PDF reader. You can open this document directly in your PDF reader from the Maestro Help menu, by choosing Manuals Index.

3. There are issues with the PDF reader (as described above).

## 18.5 Tutorials

Tutorial material is provided with most of the products, either in the User Manual or in a separate Quick Start Guide. The tutorials come with input structures, which are kept in zip files in `$/SCHRODINGER/tutorials`. You can copy the input structures and open the tutorial documentation from the Tutorials panel, which you open by choosing Help → Tutorials.

To enable you to choose a particular kind of exercise or tutorial set, the tutorials are put into one or more classes, and these classes are grouped under broader categories. You can choose the category from the Show tutorials by option menu (e.g. Modeling method), and the option menu below it is populated with the classes that belong to this category. When you make a choice from these option menus, a list of tutorials in the chosen class is displayed in the table, each with a title and a description.

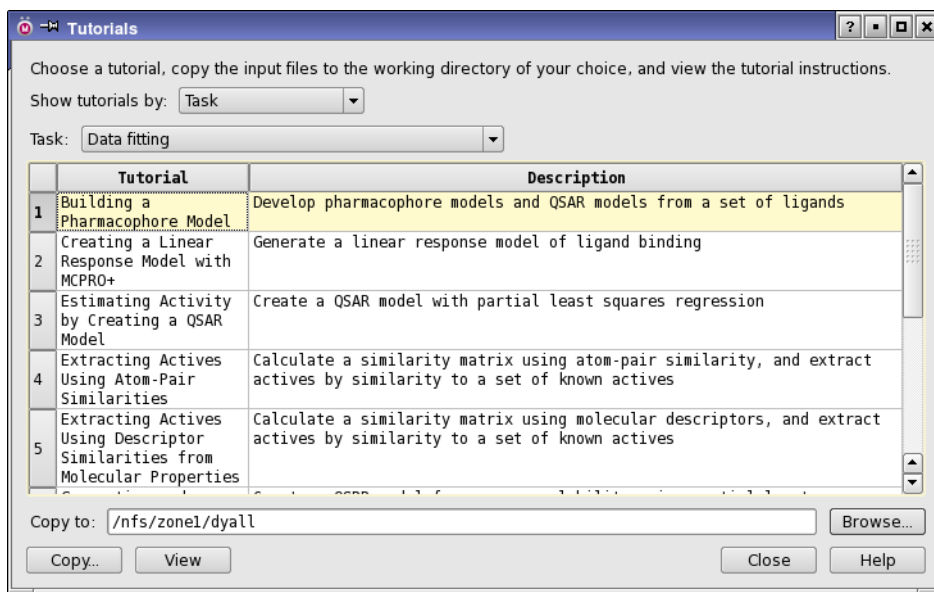


Figure 18.2. The Tutorials panel.

For example, if you choose to show tutorials by Task, the option menu below Show tutorials by is labeled Task, and you can choose from various tasks. If you choose Data fitting from this option menu, for example, a list of tutorials that involve data fitting is displayed in the table, sorted alphabetically by the tutorial title (given in the Tutorial column).

The tutorials listed can include entire Quick Start Guides or tutorial chapters in User Manuals, or individual exercises within one of these tutorials. You can then choose the tutorial that you are interested in from the table.

Once you have chosen the tutorial, you can copy the input files to your working directory. You can specify the working directory in the Copy to text box, or click Browse to navigate to the desired directory. After specifying the directory, click Copy to copy the tutorial input files to this directory, which is created if it does not exist.

To view the instructions for the tutorial, click View. If you have Adobe Reader installed, the PDF document opens at the tutorial exercise that you have chosen (which for entire manuals is the beginning of the tutorial exercises). Otherwise, the PDF document opens at the beginning, and you can use the bookmarks or the Contents to find the tutorial exercise. The title listed in the Tutorial column is usually the title of the section in the document that contains the instructions.

## 18.6 The Schrödinger Web Site

The Schrödinger web site, <http://www.schrodinger.com>, contains information about all our products. In the [Support Center](#), you can find the manuals in PDF format and known issues pages for each product. The manuals on the web site are the most up-to-date. The web site also contains information about product releases and software updates. Consult the web site for the most recent information on a product.

The web site has a knowledge base at <http://www.schrodinger.com/kb> that covers many common questions and issues, including problems and workarounds, restrictions and limitations, fixes to software issues, instructions for particular tasks, and information on specific features of the software. You can search the knowledge base from this page, or you can use your favorite search engine, and include Schrodinger in the search terms.

## 18.7 Technical Support

If you have questions that are not answered from any of the above sources, contact Schrödinger using the information below.

Web: <http://www.schrodinger.com/supportcenter>  
E-mail: [help@schrodinger.com](mailto:help@schrodinger.com)  
Mail: Schrödinger, 101 SW Main Street, Suite 1300, Portland, OR 97204  
Phone: +1 503 299-1150 (USA, 9am – 5pm Pacific Time)  
+49 621 438-55173 (Europe, 9am – 5pm Central European Time)  
Fax: +1 503 299-4532 (USA, Portland office)  
FTP: <ftp://ftp.schrodinger.com>

Generally, using the web form is best because you can add machine output and upload files, if necessary. You will need to include the following information:

- All relevant user input and machine output
- Maestro purchaser (company, research institution, or individual)
- Primary Maestro user
- Installation, licensing, and machine information as described below.

The instructions below describe how to gather the required machine, licensing, and installation information, and any other job-related or failure-related information, to send to technical support. Where the instructions depend on the profile used for Maestro, the profile is indicated.

### For general enquiries or problems:

1. Open the Diagnostics panel.
  - **Maestro:** Help → Diagnostics
  - **Windows:** Start → All Programs → Schrodinger-2014-3 → Diagnostics
  - **Mac:** Applications → Schrodinger2014-3 → Diagnostics
  - **Command line:** `$SCHRODINGER/diagnostics`
2. When the diagnostics have run, click Technical Support.

A dialog box opens, with instructions. You can highlight and copy the name of the file.

3. Attach the file specified in the dialog box to the web form.

If you have already submitted a support request, use the upload link in the email response from Schrödinger to upload the file. If you need to submit a new request, you can attach the file when you fill in the form.

**If your job failed:**

1. Open the Monitor panel, using the instructions for your profile as given below:

- **Maestro/Jaguar/Elements:** Tasks → Monitor Jobs
- **BioLuminate/MaterialsScience:** Tasks → Job Monitor

2. Select the failed job in the table, and click Postmortem.

The Postmortem panel opens.

3. If your data is not sensitive and you can send it, select Include structures and deselect Automatically obfuscate path names.

4. Click Create.

An archive file is created in your working directory, and an information dialog box with the name of the file opens. You can highlight and copy the name of the file.

5. Attach the file specified in the dialog box to the web form.

If you have already submitted a support request, use the upload link in the email response from Schrödinger to upload the file. If you need to submit a new request, you can attach the file when you fill in the form.

6. Copy and paste any log messages from the window used to start the interface or the job into the web form (or an e-mail message), or attach them as a file.

- **Windows:** Right-click in the window and choose Select All, then press ENTER to copy the text.
- **Mac:** Start the Console application (Applications → Utilities), filter on the application that you used to start the job (Maestro, BioLuminate, Elements), copy the text.

**If Maestro failed:**

1. Open the Diagnostics panel.

- **Windows:** Start → All Programs → Schrodinger-2014-3 → Diagnostics
- **Mac:** Applications → SchrodingerSuite2014-3 → Diagnostics
- **Linux/command line:** `$SCHRODINGER/diagnostics`

2. When the diagnostics have run, click Technical Support.

A dialog box opens, with instructions. You can highlight and copy the name of the file.

3. Attach the file specified in the dialog box to the web form.

If you have already submitted a support request, use the upload link in the e-mail response from Schrödinger to upload the file. If you need to submit a new request, you can attach the file when you fill in the form.

4. Attach the error files to the web form.

The files should be in the following location:

- **Windows:** %LOCALAPPDATA%\Schrodinger\appcrash  
(Choose Start → Run and paste this location into the Open text box.)  
Attach `maestro_error_pid.txt` and `maestro.exe_pid_timestamp.dmp`.
- **Mac:** \$HOME/Library/Logs/CrashReporter  
(Go → Home → Library → Logs → CrashReporter)  
Attach `maestro_error_pid.txt` and `maestro_timestamp_machinename.crash`.
- **Linux:** \$HOME/.schrodinger/appcrash  
Attach `maestro_error_pid.txt` and `crash_report_timestamp_pid.txt`.

# The Maestro File Format

All Schrödinger products use the Maestro file format as their primary method of storing molecular structure information. The Maestro file format is extensible. That is, users and third-party programs can add additional fields that will be accepted and retained when the files are read by Schrödinger products. Maestro files are also self-describing; data items are named rather than simply identified by position, and the data type (string, real number, integer and Boolean) is included as a single-digit code letter at the beginning of each data name.

Since Maestro files can accept additional user-defined fields, it is not possible to give an all-inclusive example of a Maestro file. Instead, this appendix gives a general overview of the Maestro file format and describe the components used for most Schrödinger applications.

## A.1 Basic File Description

Maestro format files are free-format ASCII text. All white space (spaces, tab characters, end of lines etc.) is ignored. Schrödinger applications will write files in a consistent layout in order to enhance human readability but the files are not, in fact, required to follow this layout. Except for the requirement that string type data items which contain blanks be surrounded by double quotes, there are no restrictions, such as width or precision of the numeric fields, on the data items.

## A.2 Data Blocks

The basic unit of a Maestro file is a block, a series of data items contained within a pair of curly braces { }. For instance, the following is the first block of the example file in shown in this appendix:

```
{
  s_m_m2io_version
  :::
  1.0.0
}
```

Most blocks in the Maestro file are preceded by a name, for example, `f_m_ct`, where ‘f’ stands for ‘full’ (see below), ‘m’ generally stands for ‘Maestro’ because the data originated from Maestro, and ‘ct’ stands for ‘CT’—short for ‘Connection Table’, which can generally be thought of as a collection of atoms.

Blocks can be nested within other blocks, and if a block contains a list of data values, the block may be indexed. That is, the number of data values contained in the block can be appended to the name. Indexed blocks are identified by having names of the form: 'name[<number of items>]'. For example, the file shown in [Section A.5](#) contains an indexed block of the name `m_atom[18]`. In this block name, 'm' means that the data originated in Maestro, 'atom' means that the data values included in the block belong to atoms, and '18' indicates that there are 18 sets of data in the indexed block (representing 18 atoms).

Within each block there are two sections: a list of the names corresponding to the data fields included in each data item, and the actual data items. In the example file, the first three data field names in the `m_atom[18]` block are:

```
i_m_mmod_type  
r_m_x_coord  
r_m_y_coord
```

The end of the first section is denoted by a separator ' ::: ', and followed by the actual data items. In the example file, the first three data items are:

```
1 3 0.547623 1.262401 -0.990300 1 " " X " " 2  
0.00000 0.00000 CHEX " " " " 6 0 0 1 ""  
2 3 -0.930177 1.296701 -1.411700 1 " " X " " 2  
0.00000 0.00000 CHEX " " " " 6 0 0 1 ""  
3 3 -1.821477 1.772701 -0.253300 1 " " X " " 2  
0.00000 0.00000 CHEX " " " c1" 6 0 0 1 ""
```

There must be the same number of data values as there are data names, and the fields within the data items must appear in the same order as the data names are listed. In the above example, for instance, the first field in the first line of data ('1') is the index number. The second number ('3') is the MacroModel atom type, indicated by the data name `i_m_mmod_type`. Index numbers are required in an indexed block and do not count against data names.

The end of the data item section is indicated by a second ' ::: ' separator. A file may contain any number of structures (CT blocks), and each structure block may contain any number of atom and bond data items.



## A.3 Compressed Format

Files may use a compressed format, most commonly when storing information for a set of conformers. In a compressed file, the first CT block must be a “full” block containing all the information described above. The name of this block is 'f\_m\_ct'. This full block can be followed by any number of “partial” CT blocks with the name 'p\_m\_ct'. The partial blocks contain only information which is different from that in the last preceding full CT block. For example, a file of conformers will have only one copy of the bond table (the m\_bond[36] block in the example file), and it will be stored in the full CT. Subsequent partial CT blocks will read bond information from the preceding full CT block.

## A.4 Data Item Names

The names of data items in a Maestro format file follow a convention which allows the type of the data item and the “owner” of the data to be identified. Names have the form 't\_o\_d', where t is the type descriptor, o is the “owner” and d is the actual data name. For instance, the first data name in the m\_bond[36] block is 'i\_m\_mmod\_type'. The first character of the name represents the data type. The acceptable types are:

i – integer	s – string value
r – real number	b – Boolean value

Owner values indicate the application from which the data item most likely originated. Including this field in the data name allows multiple applications to store identically titled quantities. For instance, two applications could store data fields named “energy.” Currently, basic geometrical and connectivity information, which is shared by most Schrödinger applications, have 'm' (for Maestro) owner fields. Data introduced by MacroModel have 'mmod' owner fields, data introduced by QikProp have 'qp' owner fields.

In the 'i\_m\_mmod\_type' example, 'i' indicates the value in the corresponding data field is an integer. The letter 'm' in the owner field means that the data originated from Maestro, and 'mmod\_type' is an abbreviation for “MacroModel atom type,” which is what the data field represents.

## A.5 Example Maestro File

Below is extract from a Maestro format file. The complete file is not shown. Where data has been exempted, it has been noted with an ellipse (...). The text in italic type is provided as annotation and is not a part of the file.

The first block in the file is unnamed. This contains required information that is relevant to the whole file.

```
{  
  s_m_m2io_version  
  :::  
  1.0.0  
}
```

f_m_ct {	The "CT" block. Each structure in the file is contained in such a block. This is a full block.
s_m_title	The only CT-level data name. A string value representing the title of this structure.
:::	The separator between the data names and data values.
"Cyclohexane"	The value of the "title" data item.
m_atom[18] {	The start of the atom block for this CT block. There are 18 atoms in this block.
i_m_mmod_type	The MacroModel atom type.
r_m_x_coord	The X-coordinate.
r_m_y_coord	The Y-coordinate.
r_m_z_coord	The Z-coordinate.
i_m_residue_number	The residue number.
s_m_insertion_code	The PDB insertion code.
s_m_mmod_res	The one-letter MacroModel residue code.
s_m_chain_name	The PDB chain name.
i_m_color	The color for this atom.
r_m_charge1	The partial atomic charge.
r_m_charge2	The partial atomic charge.
s_m_pdb_residue_name	The PDB residue name.
s_m_pdb_atom_name	The PDB atom name.

<code>s_m_grow_name</code>	<i>The name used by the Maestro structure builder.</i>
<code>i_m_atomic_number</code>	<i>The atomic number.</i>
<code>i_m_formal_charg</code>	<i>The formal charge.</i>
<code>i_m_representation</code>	<i>The representation used to draw this atom.</i>
<code>i_m_visibility</code>	<i>A flag to indicate whether this atom is displayed in Maestro or not.</i>
<code>s_m_atom_name</code>	<i>The user-specified atom name.</i>
<code>:::</code>	<i>The separator for the end of the data items.</i>

Next follow the data values. The first column contains an index number that is assigned automatically. Remaining columns represent the data values in the same order as data names given above.

```

1  3  0.547623  1.262401  -0.990300  1 " " X " "  2  0.00000
0.00000 CHEX " " " "  6  0  0  1  ""

2  3  -0.930177  1.296701  -1.411700  1 " " X " "  2  0.00000
0.00000 CHEX " " " "  6  0  0  1  ""

3  3  -1.821477  1.772701  -0.253300  1 " " X " "  2  0.00000
0.00000 CHEX " " " c1" 6  0  0  1  ""

4  3  -1.624777  0.890901  0.990300  1 " " X " "  2  0.00000
0.00000 CHEX " " " "  6  0  0  1  ""

....

17 41 0.493223  -0.677999  0.001900  1 " " X " "  21  0.00000  0.00000
CHEX " " " n3"  1  0  0  1  ""

18 41 1.817023  0.395501  0.566000  1 " " X " "  21  0.00000
0.00000 CHEX " " " n2"  1  0  0  1  ""

:::  The separator for the end of the data values.
}  The end of the atoms block.

```

<code>m_bond[36] {</code>	<i>The bond block. There are 36 bonds.</i>
<code>  i_m_from</code>	<i>The atom the bond is from.</i>
<code>  i_m_to</code>	<i>The atom the bond is to.</i>
<code>  i_m_order</code>	<i>The bond order.</i>
<code>  i_m_from_rep</code>	<i>The graphical representation for the "from" half-bond.</i>

## Appendix A: The Maestro File Format

---

i\_m\_to\_rep                    *The graphical representation for the “to” half-bond.*

:::                                *The end of the data names for bond data.*

*What follows are the data items for the bond block. The first column contains an automatically assigned index number for each item.*

1    1    2    1 1 1

2    1    6    1 1 1

...

35 17    6    1 1 1

36 18    6    1 1 1

:::                                *The end of the bond data items.*

}                                    *The end of the bond block.*

}                                    *The end of the CT block.*

# Atom Types

Maestro atom types are not “hard-wired” into the program, but are read in at run-time from a file called `atom.typ`, which is installed in `$(SCHRODINGER)/mmshare-vversion/data`. We continue to use the original MacroModel atom types for most applications, but now have a mechanism for easily adding new types.

You can add your own atom types and supply parameters for these types in the force-field file. The default `atom.typ` file is the one located in `$(SCHRODINGER)/mmshare-vversion/data`. A local file of this name overrides the default, as does a local file whose name is `filename.typ`, where `filename` is the stem of the `filename.mae` file. This system of default version with local overrides is analogous to that used for force field and solvation files.

Currently Maestro accepts atom types up through number 300. We restrict the type numbers that we supply to the range 0 through 199. When adding your own types, you should begin with the number 200. Negative atom types are not accepted.

Inside Maestro you can change atoms in existing structures to new types, including user-defined types. However, no provision is made in the current version for the builder to obtain the geometric information it needs from the `atom.typ` file, which would require extensions to the format of this file. Also, the original atom types remain “hard-wired” in Maestro. Therefore, you should not attempt to redefine types which we supply. Instead, add new types. The `atom.typ` file itself contains comments describing its format and usage.

The atom types and their equivalents in other force fields are listed in [Table B.1](#) and [Table B.2](#). These atom types are defined in the `atom.typ` file. Note that 00 atoms are stored as type 0 in the atom connection table, and that all current force fields require explicit hydrogens on hetero-atoms.

## Appendix B: Atom Types

Table B.1. Atom types and equivalents.

No.	Symbol	Description	Equivalencies		
			MM2/ MM3	Charmm	Amber
1	C1	Carbon - sp			
2	C2	Carbon - sp <sup>2</sup>	2,3	CT,C	C, C*, CA, CB, CC, CM, CF, CG, CN
3	C3	Carbon - sp <sup>3</sup>	1	CT	CT
4	CA	United atom CH - sp <sup>3</sup>		CH1E	CH
5	CB	United atom CH <sub>2</sub> - sp <sup>3</sup>		CH2E	C2
6	CC	United atom CH <sub>3</sub> - sp <sup>3</sup>		CH3E	C3
7	CD	United atom CH - sp <sup>2</sup>		CR1E	CD, CE, CI, CP
8	CE	United atom CH <sub>2</sub> - sp <sup>2</sup>			
9	CF	United atom CH - sp			
10	CM	Carbanion (C <sup>-</sup> )			
11	CP	Carbocation (C <sup>+</sup> )	30		
12	CR	Carbon free radical	29		
...					
14	C0	Any carbon			
15	O2	Oxygen - double bond	7	O	O, O2
16	O3	Oxygen - single bond	6	OH1, OH2	OS, OH
17	OA	United atom OH		OH1E	
18	OM	O <sup>-</sup> (alkoxide, carboxylate)	47		OC
19	OW	United atom H <sub>2</sub> O		OH2E	
20	OP	Oxonium (sp <sup>2</sup> ) =[O <sup>+</sup> ]-			
21	OQ	Oxonium (sp <sup>3</sup> ) R <sub>3</sub> O <sup>+</sup>			
...					
23	O0	Any oxygen			
24	N1	Nitrogen - sp	10		

Table B.1. Atom types and equivalents. (Continued)

No.	Symbol	Description	Equivalencies		
			MM2/ MM3	Charmm	Amber
25	N2	Nitrogen - sp <sup>2</sup>	9	N, NR, NP, NH1, NH2	N, NB, NC, N*, N2
26	N3	Nitrogen - sp <sup>3</sup>	8	NH3	NT
27	NA	United atom NH - sp <sup>3</sup>			
28	NB	United atom NH <sub>2</sub> - sp <sup>3</sup>		NH1E	
29	NC	United atom NH - sp <sup>2</sup>			
30	ND	United atom NH <sub>2</sub> - sp <sup>2</sup>		NH2E	
31	N4	N <sup>+</sup> - sp <sup>2</sup>		NC2	NA
32	N5	N <sup>+</sup> - sp <sup>3</sup>	39		N3
33	NE	United atom NH <sup>+</sup> - sp <sup>3</sup>			
34	NF	United atom NH <sub>2</sub> <sup>+</sup> - sp <sup>3</sup>			
35	NG	United atom NH <sub>3</sub> <sup>+</sup> - sp <sup>3</sup>		NH3E	
36	NH	United atom NH <sup>+</sup> - sp <sup>2</sup>			
37	NI	United atom NH <sub>2</sub> <sup>+</sup> - sp <sup>2</sup>		NC2E	
38	NM	N <sup>-</sup> - sp <sup>3</sup>			
39	NP	N <sup>-</sup> - sp <sup>2</sup>			
40	N0	Any nitrogen			
41	H1	H-Electroneut(e.g., C,S)	5, 44	HA	HC, HS
42	H2	H-O (Neutral)	21, 24	H,HC	HO
43	H3	H-N (Neutral)	23, 28	H,HC	H, H2
44	H4	H <sup>+</sup> (Cation)	48 MM3 (none in MM2)		H3
45	H5	H <sup>-</sup> (Anion)			
...					
48	H0	Any hydrogen			
49	S1	Sulfur	15,17,18	S	S, SH
50	SA	United atom SH		SH1E	

## Appendix B: Atom Types

Table B.1. Atom types and equivalents. (Continued)

No.	Symbol	Description	Equivalencies		
			MM2/ MM3	Charmm	Amber
51	SM	S <sup>-</sup> (thiolate anion)			
52	S0	Any Sulfur		S	
53	P3	Phosphorus, trivalent	25		P
54	B2	Boron - sp <sup>2</sup>	26		
55	B3	Boron - sp <sup>3</sup>	27		
56	F0	Fluorine	11		
57	Cl	Chlorine	12		
58	Br	Bromine	13		
59	I0	Iodine	14		
60	Si	Silicon	19		
61	Du	Dummy atom for FEP			
62	Z0	Special atom to be defined			
63	Lp	Lone electron pair			LP
64	00	Any atom	0	*	
65	Li	Li <sup>+</sup>			Li
66	Na	Na <sup>+</sup>		SOD	Na
67	K0	K <sup>+</sup>		POT	K0
68	Rb	Rb <sup>+</sup>			Rb
69	Cs	Cs <sup>+</sup>		CES	
70	Ca	Ca <sup>+2</sup>		CAL	
71	Ba	Ba <sup>+2</sup>			
72	Mg	Mg <sup>+2</sup>		MG	
73	M2	Mn <sup>+2</sup>			
74	M3	Mn <sup>+3</sup>			
75	M4	Mn <sup>+4</sup>			
76	M5	Mn <sup>+5</sup>			
77	M6	Mn <sup>+6</sup>			



Table B.1. Atom types and equivalents. (Continued)

No.	Symbol	Description	Equivalencies	
			MM2/ MM3	Charmm Amber
78	M7	Mn <sup>+7</sup>		
79	f2	Fe <sup>+2</sup>		
80	f3	Fe <sup>+3</sup>		
81	o2	Co <sup>+2</sup>		
82	o3	Co <sup>+3</sup>		
83	n2	Ni <sup>+2</sup>		
84	n3	Ni <sup>+3</sup>		
85	c1	Cu <sup>+</sup>		
86	c2	Cu <sup>+2</sup>		
87	Zn	Zn <sup>+2</sup>		
88	m3	Mo <sup>+3</sup>		
89	m4	Mo <sup>+4</sup>		
90	m5	Mo <sup>+5</sup>		
91	m6	Mo <sup>+6</sup>		
92	Sr	Sr <sup>+2</sup>		
93	L0	Lithium neutral		
94	M0	Magnesium neutral		
95	As	Arsenic, pentavalent tetrahedral (e.g. AsO <sub>4</sub> <sup>3-</sup> )		
...				
100	SP	S <sup>+</sup>		
101	S2	Sulfur - sp <sup>2</sup>		
102	Cm	Cl <sup>-</sup>		CLA
103	B0	Any boron		
104	Fm	F <sup>-</sup>		
105	Bm	Br <sup>-</sup>		
106	Im	I <sup>-</sup>		

## Appendix B: Atom Types

Table B.1. Atom types and equivalents. (Continued)

No.	Symbol	Description	Equivalencies		
			MM2/ MM3	Charmm	Amber
107	P5	Phosphorus, pentavalent tetrahedral (e.g. $\text{PO}_4^{3-}$ )			
108	P0	Any phosphorus			
109	S4	Sulfur, tetravalent			
110	S6	Sulfur, hexavalent octahedral (e.g. $\text{SF}_6$ )			
111	P4	$\text{P}^+$ , tetravalent			
112	Se	Selenium			
113	ST	Sulfur, hexavalent tetrahedral (e.g. $\text{SO}_4^{2-}$ )			
114	Sm	Sulfide anion, $\text{S}^{2-}$			
115	Om	Oxide anion, $\text{O}^{2-}$			
...					
150	PI	Ligand dummy atom			

Table B.2. Generalized atom types.

No.	Symbol	Description
151	GA	Isolated atom
152	GB	Linear-single coordinate
153	GC	Linear-two coordinate
154	GD	Trigonal-two coordinate
155	GE	Trigonal-three coordinate
156	GF	Tetrahedral-three coordinate
157	GG	Tetrahedral-four coordinate
158	GH	Trigonal bipyramid-three coordinate
159	GI	Trigonal bipyramid-four coordinate
160	GJ	Trigonal bipyramid-five coordinate
161	GK	Octahedral-four coordinate
162	GL	Octahedral-five coordinate
163	GM	Octahedral-six coordinate
164	GN	Pentagonal bipyramid-seven coordinate
165	GO	Twisted cube-eight coordinate
166	GP	Nine coordinate
167	GQ	Ten coordinate
168	GR	Eleven coordinate
169	GS	Icosahedron-twelve coordinate
170	GT	Thirteen coordinate
171	GU	Fourteen coordinate
172	GV	Fifteen coordinate
173	GW	Sixteen coordinate



# Substructure Notation

This appendix describes a linear substructure notation proprietary to Schrödinger, referred to as `mmsubs`. The `mmsubs` notation is based on the linear substructure notation used in MacroModel. The implementation is independent of the MacroModel implementation, and has some extensions over the MacroModel notation, along with a few differences.

Both `mmsubs` and MacroModel notations resemble the better-known SMILES and SMARTS notations. They all involve atom type symbols, bond symbols, and other connectivity indications, such that an arbitrary topology (including branches and rings) can always be expressed in a linear pattern string.

An `mmsubs` pattern expresses a molecular substructure as a list of atoms connected by bonds. An atom can be specified either exactly, using a symbol for a specific atom type, or loosely, using a symbol encompassing multiple atom types. Similarly, a bond can be specified either exactly, using a symbol for a specific bond order, or loosely, using the wildcard bond order symbol (which covers all bond orders).

Patterns can be limited to the required atoms and bonds. In `mmsubs` pattern matching, only the atoms and bonds explicitly specified are searched for. No assumption is made about anything else that may be attached: unspecified attachments cannot disqualify a match on the explicit pattern. Pattern matching does not include checking of valency against the specified bond orders. This is not usually a problem, because illegal valencies will generally not be matched.

The syntax to represent connectivity differs somewhat from that used in SMILES and SMARTS. The support for expressing structural alternatives is also different between notations. The `mmsubs` notation is somewhat less flexible than SMILES and SMARTS, but the reduced flexibility rarely presents a serious problem.

## C.1 Atom and Bond Types

Structures expressed in `mmsubs` (or MacroModel) notation use MacroModel atom type symbols. The MacroModel atom types are listed in [Appendix B](#).

Every MacroModel atom type symbol is two characters long, and is case-sensitive. It can consist of letters and numbers, so you must be careful to distinguish between O and 0 (upper-case letter O and zero), and between l and 1 (lower-case letter L and one).

If there are multiple atom types for an element, a wildcard symbol encompassing all of the element's atom types is provided. Our convention is to spell it with the usual first letter followed by 0 (zero). For example, the wildcards to specify any carbon and any oxygen are C0 and O0, respectively. The atom type symbol 00 (two zeroes), which matches any atom type of any element. You can use 00 in mmsubs patterns where an atom specification is needed to define connectivity, but the specific type or element is irrelevant.

The bond order symbols recognized in mmsubs patterns are given in [Table C.1](#).

Table C.1. Bond order symbols in mmsubs notation

Symbol	Description
.	Zero-order bond (see Comment below)
-	Single bond
=	Double bond
≡	Triple bond
*	Any bond order (wildcard)

Zero-order bonds are used in patterns when a bond needs to be expressed, but it is not possible to define its precise nature. Some uses of zero-order bonds are:

- When the bond is in the process of being formed or broken. One example would be in the (physically non-realistic) situation of a FEP simulation. Another, more physically realistic, example is a transition state, where the bond is actually forming or breaking.
- Representation of certain metal-ligand interactions. Bonds that are significantly ionic in nature can't really be considered to have a bond order in the conventional sense.

As an example, the following mmsubs pattern specifies the essential atoms of ethyl vinyl ether:

```
C2=C2-O3-C3-C3
```

C2, O3, and C3 are the MacroModel atom type symbols for sp<sup>2</sup> carbon, non-carbonyl oxygen, and sp<sup>3</sup> carbon, respectively.

Observe the use of the bond symbol = to represent a double bond, and - for single bonds.

Thus, ethyl vinyl ether can also be specified using wildcard atom types, like this:

```
C0=C0-O0-C0-C0
```

In this pattern spec, the bond orders remain explicit. If the first bond is generalized, using a wildcard symbol,

```
C0*C0-O0-C0-C0
```

since \* can match a single, double, or triple bond, this more generalized pattern can match diethyl ether, ethyl vinyl ether, or ethoxy acetylene.

## C.2 Ring closure

Ring-forming bonds are expressed as a bond symbol followed by a number, where the number is the pattern position of the symbol for the other atom in the ring bond. For example, cyclopentane can be expressed as

```
C0-C0-C0-C0-C0-1
```

The final -1 indicates that the fifth carbon has a single bond to the atom specified at position 1 in the pattern.

Pattern positions are numbered from 1 at the leftmost atom type symbol, and increment to the right. Bond symbols (and any other punctuation) do not affect the numbering. A ring closure must be referred from right to left, that is, from an atom specified later in the pattern to an atom specified earlier. The ring-closure indications themselves are *not* counted as positions. This makes sense since a closure introduces no additional atom.

## C.3 Chain branching

To allow specification of branched structures, mmsubs accepts parenthesized pattern sections. An opening parenthesis initiates a branch, and the corresponding closing parenthesis ends the branch. A bond symbol after the closing parenthesis is tied to the atom symbol just before the opening parenthesis.

For example, methylcyclobutane could be expressed like this:

```
C0(-C0)-C0-C0-C0-1
```

The parentheses indicate that the 2nd carbon is bonded to the 1st carbon, and that the 3rd carbon is also bonded to the 1st carbon. The 5th carbon is bonded to the 1st carbon, forming a ring of 4 (not 5) carbons.

Branches off branches can be specified by nesting parenthesized sections. For example, isopropylbenzene can be expressed as

```
C0=C0(-C0(-C0)-C0)-C0=C0-C0=C0-1
```

and threonine can be expressed as

```
N0-C0(-C0(-C0)-O0-H0)-C0=O0
```

Arbitrarily deep nesting of branches is allowed.

In patterns with more complex branching, the chance of error due to unbalanced parentheses is greater. The mmsubs software treats excess closing parentheses as erroneous, but quietly accepts patterns with excess opening parentheses, and implicitly inserts the matching closing parentheses at the end of the pattern. This may not be what you intended, so you should check carefully that the parentheses match.

### C.4 Optional atoms

Optional atoms can be specified in mmsubs notation so that the substructure will match whether or not the optional atom is found. The syntax is to put the optional atom and its preceding bond symbol in square brackets. With this pattern

```
N0([-H0])-C0(-C0-O0[-H0])-C0=O0
```

serine would be identified whether or not the optional hydrogens were present in the structure searched. Note that the first optional hydrogen in that pattern is also in a chain branch, but alone. In cases like this, the parentheses should go on the outside, as above.

The square bracket syntax can only be applied to individual atoms. It cannot be applied to chains, and the usage cannot be nested. It is not permitted to specify the first atom in a pattern as optional.

### C.5 Special Cases

The MacroModel atom type C2 needs special attention. This type covers sp<sup>2</sup> carbon as it occurs both in aromatic rings and in carbonyl groups. In cases where you want to match only one C2 subtype, you need to specify an atom attached to the C2, to exclude matches on the other subtype.

For example, if an aromatic ring pattern contains C2\*C2\*C2 and it is undesirable for it to match a structure containing C2-C2(=O2)-C2 then specifying an attached atom that is *not* O2 will exclude the undesirable matches: for example, C2\*C2(-H0)\*C2 might suffice.

The most general way to exclude unwanted carbonyl matches on a C2 in an aromatic ring pattern is to require that the C2 have a single bond to an atom of any type. In this example, the pattern to use is C2\*C2(-00)\*C2.



## C.6 Examples

In this section, some more complex examples are presented. The first is norbornane, which is a bicyclic compound, and can be represented as follows:

```
C0-C0-C0-C0 (-C0-1) -C0-C0-1
```

Two ring closures are indicated, as the compound is bicyclic. In this pattern, both closures, of the bridge and of the main ring, refer to the same position. This is not required. For example, these patterns are valid and equivalent to the above:

```
C0-C0-C0-C0-C0 (-C0-2) -C0-1
```

```
C0-C0-C0-C0-C0-C0 (-C0-3) -1
```

Now note something about branches, which is actually independent of the ring closures: If you swap a parenthesized branch with the part after it, and then parenthesize the new front part, the connectivity expressed is exactly the same. For example, these two forms are equivalent:

```
C0-C0-C0-C0-C0 (-C0-2) -C0-1
```

```
C0-C0-C0-C0-C0 (-C0-1) -C0-2
```

Norbornane also provides an opportunity to emphasize one fundamental point about linear substructure representations. The appearance of some patterns may seem to imply geometric properties. The norbornane patterns above, for example, imply a 6-membered ring bridged by one atom with two bonds on either side of the ring. It is important to keep in mind that the pattern specifies connectivity only, and not geometry.

Though it would be somewhat unconventional, it is in fact possible to specify norbornane as a 5-membered ring bridged by a chain of 2 atoms, which is topologically equivalent:

```
C0-C0-C0 (-C0-C0-1) -C0-C0-1
```

```
C0-C0-C0-C0 (-C0-C0-1) -C0-1
```

```
C0-C0-C0-C0 (-C0-C0-2) -C0-1
```

```
C0-C0-C0-C0-C0 (-C0-C0-2) -1
```

```
C0-C0-C0-C0-C0 (-C0-C0-3) -1
```

Any of these patterns will give exactly the same matching as one of the more conventional representations. The point is that these patterns specify topology, not geometry.

It should be clear that there can be many valid `mmsubs` expressions to match a single, non-trivial substructure. The `mmsubs` notation does not have a canonical representation, that is, `mmsubs` has no counterpart to Unique SMILES (USMILES).

The next example is of a compound containing fused heterocyclic aromatic rings. One way to express quinoline is the following:

```
N0=C0-C0=C0-C0=C0 (-1) -C0=C0-C0=C0-5
```

In this pattern, the atom types are general and the bond orders are exact. Thus, this pattern specifies an exact resonance form, and that is the only form it will match.

As an alternative, atom types are often specified more exactly, to designate the atomic hybridizations, and wildcard bonds are used for the connectivity. For quinoline, this kind of specification could look like the following:

```
N2*C2*C2*C2*C2*C2 (*1) *C2*C2*C2*C2*5
```

This pattern matches *any* resonance form of quinoline.

Each pattern indicates a simple ring closure in branch parentheses, in the middle of the pattern. Strictly speaking, the parentheses are not needed, since the ring closure is a branch by definition. Also, since the ring closure introduces no new atom, it doesn't really need to be shielded from bonding association with the symbol after it. However, we recommend use of parentheses in such cases, to keep it clear that the atoms on either side of the ring closure indication are bonded to each other.

## C.7 Formal Charge Extensions

The `mmsubs` notation has syntax to explicitly specify formal charge on an atom, separately from what the atom type itself implies. This is an extension over the MacroModel notation.

Formal charges can be specified for any MacroModel atom type, but the usage makes the most sense when applied to a wildcard atom type. The syntax is as follows:

- i. Formal charges are specified using the `{ }` braces after an atom type symbol. The symbols “+”, “-”, and “0” are used to represent positive, negative, and no charge. Examples:

`C0{+}` — any carbon with a +1 charge

`N0{-}` — any nitrogen with a -1 charge

`O0{0}` — any neutral oxygen

- ii. An integer in the range 1-9 can be used to specify the number of formal charges:

`N0{1+}` — any nitrogen with a +1 charge

`S0{2+}` — any sulfur with a +2 charge

- iii. A question mark `?` can be used to indicate any number (1 or more) of a particular charge type:

`N0{?+}` — any nitrogen with any positive charge

`C0{?-}` — any carbon with any negative charge

It is possible to create paradoxical specifications:

```
CP{-} — negatively charged CP (atom type for carbocation)
OM{+} — positively charged OM (type for oxygen with -1 charge)
```

These would not be rejected as erroneous, but it is impossible for them to ever match anything. Formal charge syntax is especially useful in atom-typing rules.

## C.8 Atom Type Equivalence Labels

The `mmsubs` software supports the use of atom type equivalence labels in substructure patterns. Such labels are defined in a data file with a simple text format, for example:

```
# Comments begin with a "#"
CS CA CB CC
CT CA CB CC C3
CU C2 CD CE
CH CA CB CC C3 H1
```

The equivalence label comes first, followed by the atom types to be made equivalent, separated by commas or spaces. Wildcard atom types are permitted, but formal charge specifiers are not. Equivalence labels take precedence over standard atom type symbols. Equivalence labels cannot be defined recursively.

With the assignments shown above, if an `mmsubs` pattern contains the equivalence label `CT`, it will match an atom of type `CA`, `CB`, `CC`, or `C3`.

Some of the labels in this example collect united atom types with non-united types, for equivalent treatment in `mmsubs` patterns. This is clearly useful in contexts where molecule connection tables might have either form.

Any number of equivalence labels can be defined. As with standard atom type symbols, character case matters in the equivalence labels, and every label must have 2 characters. The first character is conventionally a letter; a number may be used but is not encouraged.

The default equivalence labels are defined in a data file installed with the Schrödinger software in

```
$SCHRODINGER/mmshare-vversion/data/mmsubs.ini
```

If you want to augment or override the default equivalence labels, you can copy the installed `mmsubs.ini` file and edit it. To define equivalence labels for all applications, save the copy in `$HOME/.schrodinger/mmshare`. To define equivalence labels for a particular application, save the copy in the directory from which you run the application.

## C.9 Differences between mmsubs and bmin notations

For the record, here are the known technical differences between the mmsubs and bmin notations --

- In MacroModel notation, a pattern is limited to at most 50 atoms, and a maximum of 130 characters. In mmsubs notation, there is no explicit limit on the number of atoms in a pattern, though there is a limit on the pattern specification itself of about 10,000 characters.
- In MacroModel notation, the wildcard bond order symbol \* does not cover zero-order bonds. In mmsubs notation, it does.
- The MacroModel notation has no syntax for explicitly specifying formal charges.
- In MacroModel notation, equivalence labels are defined in force field data files. In mmsubs notation, equivalence labels are defined in a distinct data file.
- In MacroModel, wildcard atom type symbols are not permitted on the right-hand side of equivalence label definitions.

## C.10 Related Files

The data file that formally specifies MacroModel atom type symbols is installed in the Schrödinger software installation at the following location:

```
$SCHRODINGER/mmshare-vversion/data/atom.typ
```

Details of the atom types are given in this file. Further information on the atom types can be found in the atom-typing rules file, which is installed at the following location:

```
$SCHRODINGER/mmshare-vversion/data/mmatype.ini
```

This file uses the mmsubs notation to define the rules.

Another related file is the file that defines the default equivalence labels that can be used in mmsubs patterns,

```
$SCHRODINGER/mmshare-vversion/data/mmsubs.ini
```

You may on occasion need to override this installed file with your own customized version.

# Project Utilities

Schrödinger software is distributed with a number of utility programs and scripts that can be used in conjunction with any of the computational programs. These UNIX utility programs are installed in `$(SCHRODINGER)/utilities` (with one exception). A complete list of utilities is given in the *Schrödinger Utilities* quick reference. The general-purpose utilities are described in the *General Utilities* reference. This appendix lists utilities for Maestro project management.

UNIX conventions are used for the command syntax—see [page xix](#) for more information.

## D.1 project\_convert

This utility converts a project to the current version (project facility 2.4, Maestro 9.9). This utility is run automatically from Maestro, under Job Control, when you open a project from a previous release. The syntax is:

```
project_convert [options] input_project output_project
```

If the input and output project names are the same, the input project is overwritten. The options are given in [Table D.1](#).

Table D.1. Options for the `project_convert` command.

Option	Description
-d	Convert version down to previous version. Converts projects from Suite 2011 (version 2.4) to Suite 2010 (version 2.3)
-c	Compress the destination project as <code>.prj.zip</code> This option is currently available only with -d.
-h	Show usage summary.
-s <i>mode</i>	Specify whether to save in compressed or uncompressed form or both: <small>small</small> save in compressed form only <small>medium</small> save in uncompressed form only <small>large</small> save in compressed and uncompressed form
-WITHJC	Run under Job Control. Standard Job Control options are accepted with this option—see <a href="#">Section 2.3</a> of the <i>Job Control Guide</i>

## D.2 project\_create

This utility creates a project using specified structure files. The syntax is:

```

$SCHRODINGER/run project_create structure-file [-t type] project.prj
$SCHRODINGER/run project_create -f file-list [-t type] project.prj
$SCHRODINGER/run project_create -d dir [-l type] project.prj

```

The project name must include the .prj extension. The options are given in [Table D.2](#).

Table D.2. Options for the project\_create command.

Option	Description
-d <i>dir</i>	Import all Maestro, PDB, and SD files from the specified directory
-f <i>file-list</i>	Comma separated list of files to import. If spaces appear anywhere in the names or after commas, surround with double quotes—for example "my ligands.mae", or "file1, file2, file3". Maestro files can be gzipped files (.maegz or .mae.gz).
-l <i>type</i>	Limit imports from a directory to files of the specified type. Valid types are mae, pdb, sd, and sdf. Only used with -d.
-t <i>type</i>	Ignore file extensions and assume all files are of the specified type. Valid types are mae, pdb, sd, and sdf. Only used with -f.

## D.3 project\_append

This utility appends the structures in the specified structure files to a project. The syntax is:

```

$SCHRODINGER/run project_append structure-file [-t type] project.prj
$SCHRODINGER/run project_append -f file-list [-t type] project.prj
$SCHRODINGER/run project_append -d dir [-l type] project.prj

```

The project name must include the .prj extension. The options are given in [Table D.3](#).

Table D.3. Options for the project\_append command.

Option	Description
-d <i>dir</i>	Import all Maestro, PDB, and SD files from the specified directory
-f <i>file-list</i>	Comma separated list of files to import. If spaces appear anywhere in the names or after commas, surround with double quotes—for example "my ligands.mae", or "file1, file2, file3".

Table D.3. Options for the `project_append` command.

Option	Description
<code>-l type</code>	Limit imports from a directory to files of the specified type. Valid types are <code>mae</code> , <code>pdb</code> , <code>sd</code> , and <code>sdf</code> . Only used with <code>-d</code> .
<code>-t type</code>	Ignore file extensions and assume all files are of the specified type. Valid types are <code>mae</code> , <code>pdb</code> , <code>sd</code> , and <code>sdf</code> . Only used with <code>-f</code> .

## D.4 project\_extract

This utility extracts usable data from a corrupted Maestro project. The syntax is:

```
project_extract -i corrupted-project.prj -o new-project.prj
[-e data-types]
```

where `-i` and `-o` specify the path to the corrupted project and the path to the new project. If `-e` is not used, the utility only attempts to extract the entry data (including properties). If `-e` is used, it must be followed by a quoted, comma-separated string listing the data types to attempt to extract, from the following types:

<code>all</code>	Attempt to extract all data types
<code>auxiliarydata</code>	Auxiliary data for entries. Includes things like trajectories, vibrations, surfaces, Phase hypotheses, etc.
<code>jobsdata</code>	Job-related information for applications you have run
<code>plotxy</code>	XY plots of Project Table entry properties
<code>primex</code>	PrimeX data
<code>psp</code>	Prime data
<code>phase</code>	Phase data
<code>strike</code>	Strike data
<code>userdata</code>	User data
<code>vcs</code>	CombiGlide data

## D.5 project\_version

This utility lists the Maestro version and release that could have produced a project. The syntax is:

```
project_version project1 [project2 ...]
```

Each project is listed with the Maestro version and the release name in parentheses. If the project has ben converted from one format to another, the version for the latest format is reported.



# Property Names

Properties of entries have two names: an internal name and a display name, or visible name. The display name is the name that is shown in the headings of the Project Table columns. Properties also belong to a “family”, and the family name is shown in menus used for property selection.

The internal name is the name used by Maestro to identify the property, and is the name that is written to and read from Maestro files. The internal name has the format *type\_author\_label*. The *type* is a single character, which identifies the variable as an integer (i), a real number (r), a string (s), or a Boolean (b). The *author* identifies the program that generated the property, or more generally the source of the property. Finally, the *label* gives information about the property itself. For example, *s\_m\_title* is the internal name of a string property generated by the author *m*, which stands for Maestro, that is the title of the entry.

When the internal name is parsed by Maestro, it is split into the three pieces. The *type* is used to assign a variable internally to store the property value. The *author* is mapped to the “family” name, and the *label* is mapped to the display name. Maestro has a table of mappings of the *author* to the family names and of the *label* to the display names. If there is no entry for *label* in the map, then the display name is constructed by replacing any underscores in *label* with spaces: thus, if the *label* is *My\_property*, the display name is *My property*. Likewise, *author* is displayed as is for the family name if it has no entry in the map. A list of authors and their mappings is given in [Table E.1](#). The list of property names is much larger, and is not given here. The display names are stored as part of the project.

The display name and the internal name can both be changed within a Maestro session—see [Section 9.11.8 on page 235](#). The display name is used only in the project. It is the internal name that is exported when you export structures. If you want to export a property with a new name (for example to an SD file), you can create a new property, and copy the desired property to the new property for export. The author for the new property in this case is *user*, by default. You can change the author, but since the author and type are stripped out when exporting to an SD file, the author is not relevant in this case.

For SD properties, you can protect the underscore characters so that they are displayed in the Project Table by preceding them with backslash characters.

Atom properties also have an internal name and a display name. The internal name has the same format as the entry properties, and the display name is derived in the same way as for entry properties that do not have a mapping, i.e. the *type* and the *author* are stripped off, and

## Appendix E: Property Names

any remaining underscores are replaced by spaces. The display name for atom properties is shown in option menus for selection of an atom property, for example.

Table E.1. Mappings for the author field in the internal name.

<b>Author</b>	<b>Family Name</b>	<b>Author</b>	<b>Family Name</b>
canvas	Canvas	mopac	MOPAC
comngen	CombiGlide	pdb	PDB
des	Desmond	phase	Phase
epik	Epik	ppw	Protein Preparation Wizard
glide	Glide	psp	Prime
glideres	Glide Residue Interactions	pspIFD	Induced Fit
i	Impact	px	PrimeX
ionizer	Ionizer	qp	QikProp
j	Jaguar	qpld	QPLD
lp	LigPrep	qs	QSite
lsbd	LSBD	sd	SD
m	Maestro	sitemap	SiteMap
mcp	MCPRO+	strike	Strike
mmod	MacroModel	user	Added by user

---

# Glossary

**ASD**—Atom Selection dialog box.

**ASL**—Atom Specification Language.

**button menu**—The menu available from a toolbar menu button, which you open by holding down the left mouse button.

**clipping planes**—The planes that define the displayed depth of the structure. Atoms are clipped (not displayed) if they are in front of the front clipping plane or behind the back clipping plane. The position of these planes is displayed in the clipping planes window.

**current working directory**—the directory that is used to write job files (the [job launch directory](#)) and the directory that is used by default in file selectors for reading and writing files. Also called the working directory.

**entry**—A structure or set of structures and associated properties. Entries are represented as a row in the Project Table, and can be used as input for jobs.

**ESL**—Entry Specification Language.

**exporting**—Writing structures and their associated data from a Maestro project to a structure file, or writing data from a Maestro project to a spreadsheet file.

**filter**—An ESL expression that is used to select, or filter, entries in the Project Table.

**grow bond**—The bond that is replaced when you add a fragment to a structure in Grow mode. The grow bond is displayed as a green arrow in the Workspace.

**importing**—Reading structures and their associated data from a structure file into a Maestro project, or reading data from a spreadsheet file into a Maestro project.

**inclusion**—Display of entries in the Workspace. Multiple entries can be included in the Workspace. The inclusion state (included, excluded, or fixed) is indicated in the In column of the Project Table.

**isovalue**—the value of a property that defines a surface. The property is a function of the three spatial coordinates, and is represented as a set of points on a three-dimensional grid.

**job directory**—The directory that is used to write temporary files for a job. Also known as the temporary directory or the scratch directory for a job. This directory is created for the job and removed at the end of the job, unless options are set to preserve it.

**launch directory**—The directory that is used to write input files for a job, and to which the output files from a job are copied when the job finishes.

**Maestro resources directory**—the directory (folder) that contains the default resource files used by Maestro. This directory is the `maestro-vversion/data/res` directory of your Schrödinger software installation.

**Maestro user resources directory**—the directory (folder) in which resource files for Maestro are kept that are specific to a user, rather than for general use. This directory is defined as follows

**Linux, Mac:**     `$HOME/.schrodinger/maestrovv`

**Windows:**     `%APPDATA%\Schrodinger\maestrovv`

where *vv* is the two-digit Maestro version number (92 for this release). `$HOME` is usually set to `/home/username` on Linux and `/Users/username` on Mac OS X. `%APPDATA%` is the location of shared data on Windows, `C:\Users\username\AppData\Roaming`.

**menu button**—A toolbar button that has a menu, which you open by holding down the left mouse button. The button has a black triangle in the lower right corner.

**option menu**—A drop-down menu from which you can select an option. Clicking the button on the menu displays the menu without having to hold down the left mouse button.

**picking**—Selecting atoms in the Workspace.

**profile**—(1) a named set of customizations of Maestro; (2) the directory (folder) in which resource files for Maestro are kept that are specific to a Maestro profile, for example, menu and toolbar customization files. This directory is the `profile/profile-name` subdirectory of your Maestro user resources directory.

**Linux, Mac:**     `$HOME/.schrodinger/maestrovv/profiles/profile-name`

**Windows:**     `%APPDATA%\Schrodinger\maestrovv\profiles\profile-name`

**project**—A collection of related data, such as structures with their associated properties. The project may include data that does not appear in the Project Table.

**Project Table**—The table that displays the contents of a project, with rows of entries and columns of properties. The table is located in the Project Table panel.

**selection**—(1) A group of atoms in the Workspace that has been picked or otherwise chosen. The selection is highlighted by markers when the appropriate option is selected. (2) A group of entries in the Project Table. The entries are highlighted in the table.

**shortcut menu**—The menu that is displayed when you right-click and hold on a component of a panel, such as the sequence viewer in the main window.

**startup directory**—The directory from which Maestro was started, on Linux (or from the command line on Mac). On Windows and Mac, there isn't a concept of a startup directory for an application, so it is set to the Schrodinger folder in your Documents folder.

**synchronization**—updating the project with changes made in the Workspace. The default is to perform synchronizations automatically.

**user profiles directory**—the directory (folder) in which Maestro profiles are kept for a specific user.

**Linux, Mac:**     \$HOME/.schrodinger/maestrovv/profiles

**Windows:**     %APPDATA%\Schrodinger\maestrovv\profiles

**user resources directory**—the directory (folder) in which resource files are kept for a specific user.

**Linux, Mac:**     \$HOME/.schrodinger

**Windows:**     %APPDATA%\Schrodinger

**volume**—a set of data points on a three-dimensional grid for a property that is a function of the three spatial coordinates.

**working directory**—*see* [current working directory](#).

**Workspace**—The open area in the center of the Maestro main window in which structures are displayed.



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120 West 45th Street  
17th Floor  
New York, NY 10036

155 Gibbs St  
Suite 430  
Rockville, MD 20850-0353

Quatro House  
Frimley Road  
Camberley GU16 7ER  
United Kingdom

101 SW Main Street  
Suite 1300  
Portland, OR 97204

Dynamostraße 13  
D-68165 Mannheim  
Germany

8F Pacific Century Place  
1-11-1 Marunouchi  
Chiyoda-ku, Tokyo 100-6208  
Japan

245 First Street  
Riverview II, 18th Floor  
Cambridge, MA 02142

Zeppelinstraße 73  
D-81669 München  
Germany

No. 102, 4th Block  
3rd Main Road, 3rd Stage  
Sharada Colony  
Basaveshwaranagar  
Bangalore 560079, India

8910 University Center Lane  
Suite 270  
San Diego, CA 92122

Potsdamer Platz 11  
D-10785 Berlin  
Germany

**SCHRÖDINGER**