Maestro 7.0

User Manual

Schrödinger Press

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January 2005

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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.

Table 3.1.

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

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.

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 all of Schrödinger's computational programs: FirstDiscovery™ (Glide™, Impact™, Liaison™, and QSite™), Jaguar™, LigPrep™, MacroModel®, Phase™, Prime™, QikProp™, and Strike™. 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.

The Maestro interface uses the OpenGL graphics tools, and can take advantage of hardware graphics capabilities, including stereo viewing capabilities. Maestro runs on SGI and Linux platforms. For information on Maestro requirements, software and hardware, see the *Schrödinger Product Installation Guide*. For information on configuring stereo viewing, see Section 11.4 on page 152.

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.

The use of this version of Maestro should be cited in publications as:

> Maestro 7.0, Schrödinger, LLC, New York, NY, 1999–2005.

This chapter provides an overview of Maestro—the general interface design, starting and ending a Maestro session, the main window and its features, Maestro projects and workflow, and running jobs from Maestro.

1.1 Starting Maestro

Before starting Maestro, you must set the `SCHRODINGER` environment variable to point to the installation directory. You can set this variable by entering the following command at a shell prompt:

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`

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

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

If you add the $SCHRODINGER directory to your path, you only need to enter the command maestro.

The options for the maestro command are listed in Table 1.1. The optional *filename* specifies a file in Maestro or MacroModel format.

Table 1.1. Options for the maestro *command*

Option	Description
-b *PDB-file*	Read a PDB file. Cannot be used with -m.
-c *command-script*	Run the specified Maestro command script when Maestro starts.
-h	Print a usage message, but do not start Maestro.
-m *filename*	Load structures from a Maestro (.mae) or MacroModel (.dat) structure file. Cannot be used with -b. The -m can be omitted if this option is at the end of the option list.
-p *project*	Load the specified Maestro project.
-s *number*	Specify the first structure to load when a Maestro file is specified for loading.
-t *number*	Specify the total number of structures to load when a Maestro file is specified for loading.
-v	Display the Maestro version number, but do not start Maestro.
-I	Display extra information about X visual settings when Maestro starts.
-SGL	Use the Schrödinger-supplied OpenGL library. The default is to use the system OpenGL library.

The directory from which Maestro was started becomes Maestro's current working directory, and all data files are written to and read from this directory unless otherwise specified (see Section 11.2.3 on page 146). You can change directories by entering the following command, either at the shell prompt before you start Maestro, or in the command input area of the Maestro main window:

`cd` *directory_name*

where *directory_name* can be either a full path or a relative path.

To find the command input area, see Figure 1.1 on page 6.

1.2 General Interface Design

The Maestro interface 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.

1.2.1 Maestro Windows

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.

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, and allow you to open the help viewer.

1.2.2 Mouse Functions

Maestro supports common mouse functions:

- The left button 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 is used for opening a 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 with the middle mouse button on the boundary of a row or column resizes the row or column.

If you have the handedness on your mouse set to "left," the mouse functions are the mirror image of those described: the right mouse button is used for picking, and the left button is used for context-sensitive menus.

If you have a two-button mouse, ensure that it is configured for three-button mouse simulation. Then the middle mouse button is simulated by pressing or holding down both buttons.

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. See the table below for a summary and Chapter 6 for more detailed information.

Table 1.2. Mapping of Workspace operations to mouse actions.

Mouse Button	Keyboard	Motion	Action
Left		click, drag	Select
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
Middle		drag highlighted parameter	Adjust bond, angle or dihedral (see Section 3.7.1 on page 43)
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

1.3 The Maestro Main Window

The Maestro main window is shown in Figure 1.1. The following main window components are always visible:

- **Title bar**—displays the project name and the current working directory
- **Auto-Help**—automatically displays context-sensitive help
- **Main menu bar**—provides access to panels
- **Workspace**—displays molecular structures

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

- **Clipping planes window**—displays a small, top view of the Workspace and shows the clipping planes and viewing volume indicators
- **Toolbar**—contains buttons for many common tasks and also provides tools for displaying and manipulating structures, as well as organizing the Workspace
- **Status bar**—displays information about a particular atom, or about structures in the Workspace, depending on where the cursor pauses:
    - **Atom**—displays the chain, residue number, element, PDB atom name, formal charge, and title or entry name (this last field is set by choosing Preferences from the Maestro menu and selecting the Feedback folder)
    - **Workspace**—displays the number of atoms, entries, residues, chains, and molecules in the Workspace
- **Sequence viewer**—shows the sequences for proteins displayed in the Workspace
- **Command input area**—provides a place to enter Maestro commands. This feature is hidden by default. To display it, choose Command Input Area from the Display menu.

You can show or hide the toolbar, the status bar, and the sequence viewer by clicking their collapse buttons:

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 toolbar).

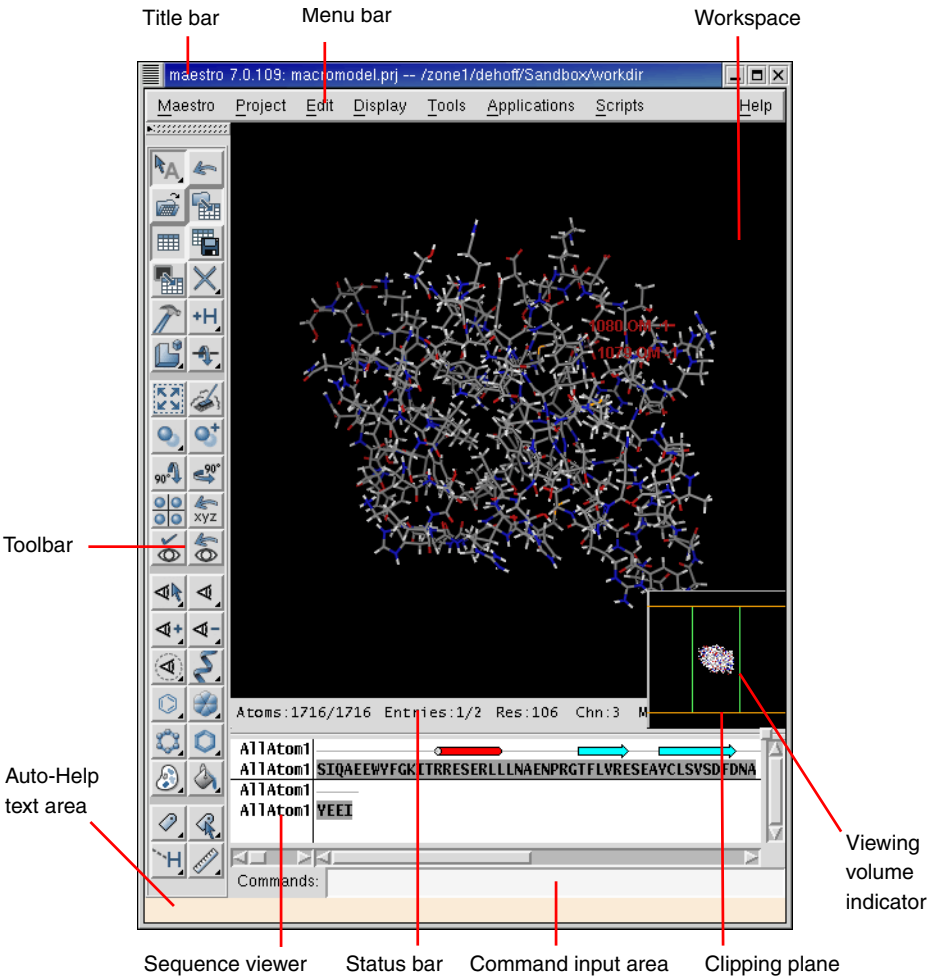


Figure 1.1. The Maestro main window.

1.3.1 The Menu Bar

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

- Maestro—save or print images in the Workspace, enter system commands, save or load a panel layout, set preferences, set up Maestro command aliases, and quit Maestro.
- Project—open and close projects, import and export structures, make a snapshot, and annotate a project. These actions can also be performed from the Project Table panel. For more information on projects, see Chapter 7.

- Edit—undo actions, build and modify structures, define command scripts and macros, and find atoms in the Workspace.
- Display—control the display of the contents of the Workspace, arrange panels, and display or hide main window components.
- Tools—group atoms; measure, align, and superimpose structures; 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 the task to be performed.
- Scripts—manage and install Python scripts that come with the distribution and scripts that you create yourself. For details, see Section 12.1 on page 157.
- Help—open the Help panel and display or hide Balloon Help (tooltips).

1.3.2 The Toolbar

Button Types

The main toolbar contains 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.

Types of Items in a Button Menu

There are four types of items on button menus, and all four types can be on the same menu (see Figure 1.2):

- **Action**—Perform an action immediately.
- **Display**—Open a panel or dialog box.
- **Object Type**—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.

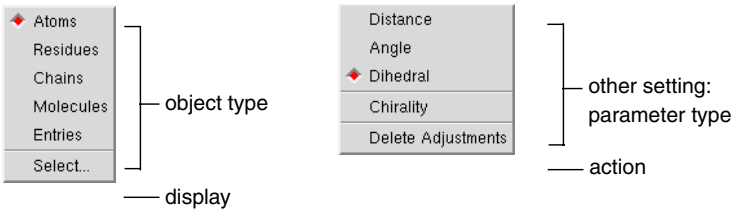


Figure 1.2. The Workspace selection ***button menu and the*** Adjust distances, angles or dihedrals ***button menu.***

The object type is marked on the menu with a red diamond and the button is indented to indicate the action to be performed.

- **Other Setting**—Set a state, choose an attribute, or choose a parameter type and click on an atom in the Workspace to act upon that parameter.

The Toolbar Buttons

The toolbar buttons are described below. Some descriptions refer to features not described in this chapter.

Workspace selection
– Choose an object type for selecting
– Open the Atom Selection dialog box

Undo/Redo
Undo or redo the last action. Performs the same function as the Undo item on the Edit menu, and changes to an arrow pointing in the opposite direction when an Undo has been performed, indicating that its next action is Redo.

Open a project
Open the Open Project dialog box.

Import structures
Open the Import panel.

Open/Close Project Table
Open the Project Table panel or close it if it is open.

Save as
Open the Save Project As dialog box, to save the project with a new name.

Create entry from Workspace
Open a dialog box in which you can create an entry in the current project using the contents of the Workspace.

Delete
– Choose an object type for deleting
– Delete hydrogens and waters
– Open the Atom Selection dialog box
– Delete other items associated with the structures in the Workspace
– Double-click to delete all atoms

Open/Close Build panel
Open the Build panel or close it if it is open.

Add hydrogens
– Choose an object type for applying a hydrogen treatment
– Open the Atom Selection dialog box
– Double-click to add hydrogens to all structures in the Workspace

Local transformation
– Choose an object type for transforming
– Open the Advanced Transformations panel

Adjust distances, angles or dihedrals
– Choose a parameter for adjusting
– Delete adjustments

Fit to screen
Scale the displayed structure to fit into the Workspace and reset the center of rotation.

Clear Workspace
Clear all atoms from the Workspace

Set fog display state
Choose a fog state. Automatic means fog is on when there are more than 40 atoms in the Workspace, off otherwise.

Enhance depth cues
Optimize fogging and other depth cues based on what is in the Workspace.

Rotate around X axis by 90 degrees
Rotate the Workspace contents around the X axis by 90 degrees.

Rotate around Y axis by 90 degrees
Rotate the Workspace contents around the Y axis by 90 degrees.

Tile entries
Arrange entries in a rectangular grid in the Workspace.

Reset Workspace
Reset the rotation, translation, and zoom of the Workspace to the default state.

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.

Display only selected atoms
– Choose an object type for displaying
– Double-click to display all atoms

Display only
– Choose a predefined atom category
– Open the Atom Selection dialog box

Also display
– Choose a predefined atom category
– Open the Atom Selection dialog box

Undisplay
– Choose a predefined atom category
– Open the Atom Selection dialog box

Display residues within N angstroms of currently displayed atoms
– Choose a radius
– Open a dialog box to set a value

Show, hide, or color ribbons
– Choose show or hide ribbons
– Choose a color scheme for coloring ribbons

Draw bonds in wire
– Choose an object type for drawing bonds in wire representation
– Open the Atom Selection dialog box
– Double-click to apply to all atoms

Draw atoms in CPK
– Choose an object type for drawing bonds in CPK representation
– Open the Atom Selection dialog box
– Double-click to apply to all atoms

Draw atoms in Ball & Stick
– Choose an object type for drawing bonds in Ball & Stick representation
– Open the Atom Selection dialog box
– Double-click to apply to all atoms

Draw bonds in tube
– Choose an object type for drawing bonds in tube representation
– Open the Atom Selection dialog box
– Double-click to apply to all atoms

Color all atoms by scheme
Choose a predefined color scheme

Color residue by constant color
– Choose a color for applying to residues
– Double-click to color all atoms

Label atoms
– Choose a predefined label type
– Delete labels

Label picked atoms
– Choose an object type for labeling atoms
– Open the Atom Selection dialog box
– Open the Composition folder of the Atom Labels panel
– Delete labels

Display H-bonds
– Choose bond type:
intra—displays H-bonds within the molecule you select
inter—displays H-bonds between the molecule you select and all other atoms in the Workspace.
– Delete H-bonds

Measure distances, angles or dihedrals
– Choose a parameter for displaying measurements
– Delete measurements

1.3.3 Shortcut Keys

Some frequently used operations in the main window have been assigned shortcut key combinations. The shortcuts, their functions, and their menu equivalents are listed in Table 1.3. Shortcut keys in the Project Table panel and the Plot panel are listed in the chapters that describe those panels.

Table 1.3. Shortcut keys in the Maestro main window

Keys	Action	Equivalent Menu Choice
CTRL+B	Open Build panel	Edit > Build
CTRL+C	Create entry	Project > Create Entry From Workspace
CTRL+E	Open Command Script Editor panel	Edit > Command Script Editor
CTRL+H	Open Help panel	Help > Help
CTRL+I	Open Import panel	Project > Import Structures
CTRL+M	Open Measurements panel	Analysis > Measurement
CTRL+N	New project	Project > New Project
CTRL+O	Open project	Project > Open Project
CTRL+P	Print	Maestro > Print
CTRL+Q	Quit	Maestro > Quit
CTRL+S	Open Sets panel	Analysis > Sets
CTRL+T	Open Project Table panel	Project > Show Table
CTRL+W	Close project	Project > Close Project
CTRL+Z	Undo/Redo last command	Edit > Undo/Redo

1.4 Maestro Workflow

In Maestro, you can either choose an action first and then select atoms, or you can select atoms first and then choose an action to perform on them.

Actions are performed either by clicking a toolbar button or opening a panel and selecting options. For details on these actions, see the section in this manual for the appropriate toolbar or panel.

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 4.

1.5 Maestro Projects

When you use Maestro, you are always working within a *project*. A project is a collection of chemical structures and their associated data. These structures and their 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 any associated

data. You can open the Project Table panel by choosing Show Table from the Project menu, or by clicking the Open/Close Project Table button on the 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.

Entries are represented by rows in the Project Table. Each row contains the row number, the title, the entry's Workspace inclusion state (the In column), a button to open the Surfaces panel if there are surfaces associated with the entry, the entry name, and any properties associated with the entry. If there are no surfaces associated with any entry, the Surf column of the Project Table is empty.

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: Glide, Jaguar, LigPrep, MacroModel, Phase, Prime, QikProp, QSite, and Strike. 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.

More information on projects is given in Chapter 7.

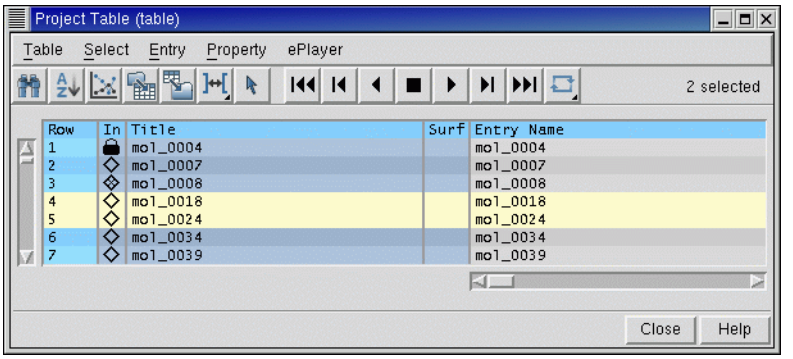


Figure 1.3. The Project Table ***panel.***

1.6 Job Launching and Incorporation

Maestro's job launching and incorporation capabilities are designed to make it easy to manage multiple structures and their passage though multiple computational programs, without having to deal with the details of the file system.

Maestro has dedicated panels for each product for preparing and submitting jobs. To use these panels, choose the appropriate product and task from the Applications menu and its submenus. Set the appropriate options in the panel, then click Start to open the Start dialog box and set options for running the job. See Section 14.2 on page 181 for a detailed description of the options in the Start dialog box. When you are finished, click Start to launch the job and open the Monitor panel.

Once a job is launched, the Monitor panel is automatically displayed and job progress is posted to the monitor window. 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 can select it in the Monitor panel and click Monitor to incorporate the results.

For more information on job control and incorporation, see Chapter 14.

Jaguar, LigPrep, MacroModel, and QikProp

These computational programs, which have been fully integrated with the Project Facility, can use Maestro structure files, single or multiple project entries and structures displayed in the Workspace as input, and can incorporate job results into the project. You can specify whether the output structures will be appended to the project, replace the input entries, or be ignored when the job finishes. As the job progresses, any interim structures are shown in the Workspace.

Some of these computational programs have additional capabilities:

- LigPrep jobs can read structures from external files. This choice of structural input has no connection with a Maestro project, so the output is required to be written to an external file.
- Jaguar maintains its own input and output files and directory structure.

FirstDiscovery

The programs comprising the FirstDiscovery suite have differing degrees of integration with the Project Facility. Glide can use selected entries from the project table as input for docking, but does not incorporate the results. The pose files that are generated are better viewed in the

Glide Pose Viewer than in the Project Table. Liaison is not integrated with the project facility at all: Liaison takes input from specified disk files or the Workspace, and the results are not incorporated. QSite and Impact are integrated into the Project Facility. Either the Workspace or a single selected entry can be used as the source of job input, and the incorporation mode can be selected. Protein preparation uses the Workspace structure as input and the resulting structures are incorporated.

For the programs that do not incorporate results, the output files are placed in the file I/O directory that you specify using the Preferences panel.

Phase

The three stages of Phase workflow behave differently in relation to the Maestro project. Development of a pharmacophore model uses structures from the project and stores information in the project, but does not incorporate results into the Project Table. Output from each step is incorporated into the next step, but not via the Project Table. Database preparation has no connection to a Maestro project. The database search automatically adds the hits to the Project Table: there are no other incorporation options.

Prime

Prime's Protein Structure Prediction works on a different model from other products. The input is a sequence rather than a structure, though the sequence can be taken from a structure in the Workspace. Output from each step is incorporated into the next step, but not via the Project Table. At the final step, the structures can be copied into the Project Table. The standalone Refinement facility is similar to MacroModel and QikProp: it takes the structure in the Workspace as input and incorporates the results into the Project Table according to the selected option.

Strike

Strike is intimately linked with the Project Facility, uses descriptor data from single or multiple Project Table entries as input, and automatically incorporates job results into the project without overwriting existing data. Workspace and selected entry molecules are used to determine which molecules are used by Strike for a given calculation. Job output can be monitored in the Monitor panel. Jobs can be run on any machine listed within the `schrodinger.hosts` file. Models generated by Strike can be imported from one project to another or exported for use at the command line.

1.7 Undoing Workspace Operations

There are two classes of operations in the Workspace: operations that act on the structure, and operations that act on the view of the molecule. The former include local transformations, other coordinate changes, and adding or removing atoms from the display. The latter include global transformations: translation, rotation, and magnification (zoom). These operations do not change the coordinates recorded in the project entry, but store a local copy that is translated, rotated, or magnified.

1.7.1 Undoing Operations on the Structures

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.

1.7.2 Undoing Operations on the View

Global molecular transformations, such as rotations and translations, cannot be undone with the Undo option on the Edit menu or in Undo Blocks. To undo such a transformation, you must save the orientation of the structure before you do the global transformation. You can also revert to the default orientation and zoom. The default orientation is defined by the coordinates of the structure. The default zoom value is the value you get by clicking the Fit to screen button on the toolbar.

To save an orientation:

- Click the Save view button in the toolbar.

To restore the saved orientation:

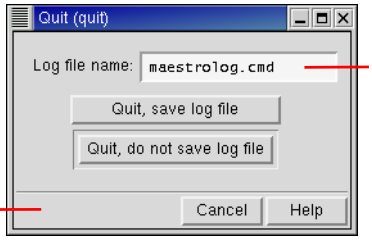
- Click the Restore view button in the toolbar.

To revert to the default orientation and zoom:

- Click the Reset workspace button in the toolbar.

1.8 Ending a Maestro Session

To end a Maestro session, choose Quit from the Maestro menu. If you want to save a log file with a record of all operations performed in the current session, click Quit, save log file on the Quit panel. This information can be useful to Schrödinger support staff when responding to any problem you report. If you do not want to save a log file, click Quit, do not save log file. If you are working in a scratch project and have not saved the project, you are prompted to do so.



Click *Cancel* to close the panel and abort the Quit operation

If you want to save a file that records the operation sequence for this Maestro session, enter a name for the file here, and then click *Quit, save log file*

Figure 1.4. The* Quit *panel.

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 selected an option not to do so). Projects are described in detail in Chapter 7. 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, PDB, Sybyl Mol2, and MDL SD format. Through the Jaguar panel, structural information can 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.

2.1 Importing Structures

Structures are imported 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 the Maestro file type, molecular representation information can be imported along with a structure. You can undo the import operation, but the changes made to the Project Table remain.

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

- Choose Import Structures from the Project menu on the main menu bar.
- Choose Structures from the Import submenu of the Table menu in the Project Table panel.
- Click the Import structures button on the main toolbar.

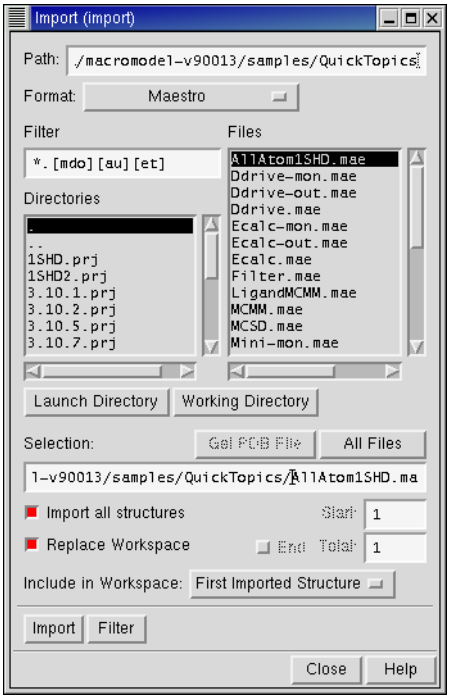


Figure 2.1. The** Import **panel.

If you have the PDB database installed, you can import a structure directly from the Import panel:

1. In the Import panel, choose PDB from the Format option.
2. Click Get PDB File and enter the PDB ID and chain name in the dialog box to copy the structure to your local directory and import it into Maestro.

Note: Unlike Maestro and SD files, PDB files do not support multiple structures, only multiple sets of coordinates for the same molecule, e.g. different NMR refinements. Certain PDB structures do not follow the PDB standard and have varying number of atoms in different MODELs. Do not import these PDB structures, as they will cause Maestro to fail.

2.1.1 Selecting Files

Selecting a file type: Before you choose files, you must specify the file type by choosing a file format from the Format menu. This choice determines the file extensions to be used, and thus the filter displayed in the Filter text box and the files displayed in the Files list.

The menu options are described below:

Maestro

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

PDB

Import PDB files, which have either a `.pdb` or a `.ent` extension. Where multiple atomic coordinates exist for a single PDB entry, Maestro chooses the atoms with the highest occupancy ratio. Properties are imported as well as structures.

Mol2

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

SD

Import MDL SD files, which have either a `.sdf` extension for multiple structure files or a `.mol` extension for files with a single structure. Properties are imported as well as structures.

Babel

Import structures from a range of other programs. The format conversion is performed by 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 other formats using Babel, you can use Jaguar to read the files. See Section 11.2.5 of the *Jaguar User Manual* for more information.The full list of file types read by Babel is included in that document.

You can also 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-v`*version*`/data/babel`

bash/ksh: `export BABEL_DIR=$SCHRODINGER/mmshare-v`*version*`/data/babel`

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

`$SCHRODINGER/mmshare-v`*version*`/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, Mopac Cartesian and Internal, and Spartan. This option is useful if you want to locate any of these kinds of structure files.

Selecting a directory: To specify the directory from which to import, you can enter it in the Path text box, navigate to it using the Directories list, or click Launch Directory or Current Directory to select the directory from which you launched Maestro or the current working directory. The path and the directory and file lists are updated for the chosen directory.

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

If you selected one of the four specific file types from the first section of the menu, or some of the Babel file types, the file that you select must have the correct extension. If you type the name of the file in the Selection text box, you must include the correct extension. In the Files list, 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 in the Format section, or select All in the Format section to view all files. You can also view files with a different extension by altering or deleting the filter and pressing RETURN or clicking Filter.

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.

2.1.2 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.

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.

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.

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.

Importing graphical information: If you import structures from a Maestro file, you can also import graphical information for the structures, such as the molecular representation. Maestro's default behavior is to read in and use this information when importing structures from a file. If you do not want imported structures to be displayed using the saved representation information, clear the Use graphical info option.

2.1.3 Error Reporting for PDB Files

When Maestro imports structures from PDB files, the color scheme it uses reflects the success or failure of the placement of bonds. Maestro 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 2.1.

Table 2.1. 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

If the placement of bonds fails, the regions of the structure in which problems were identified are colored according to the type of error. The color scheme is given in Table 2.2.

Maestro imports PDB files by running a utility, `pdbconvert`, which is described in Appendix D. The conversion creates a temporary Maestro-formatted file, and imports the structures from this file. In addition to the coloring scheme, which is set up in the temporary file, Maestro displays warning messages to indicate the status of the PDB conversion, which are listed in Table 2.3.

Table 2.2. 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.
green	A residue with an alternate location indicator. The first one listed in the PDB file is the one used to generate the converted structure.
gray	Standard residues connected by standard templates. Confidence in bond orders assigned to these residues is high.

Table 2.3. 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 *formatname* 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.

2.1.4 Entry Naming Conventions for Imported Structures

The names of entries in a project are required to be unique. Maestro enforces the uniqueness by adding suffixes to entry names to resolve any duplications. When structures are imported from a file, they are assigned entry names according to the following procedure.

- If the file already contains entry names, these names are read and used as the base of the entry name. If the file does not contain entry names, the stem of the file name (the portion before the extension) is used as the base of the entry names.
- The suffix `-imp`*n* is added to the base entry name, where *n* is a number beginning at 1, and is incremented for each import operation. Consequently, entries imported from different files automatically have different entry names.
- If the resulting entry name is not unique, the suffix `.`*m* is appended to the entry name, where *m* is a number beginning at 1, and is incremented for each import operation.

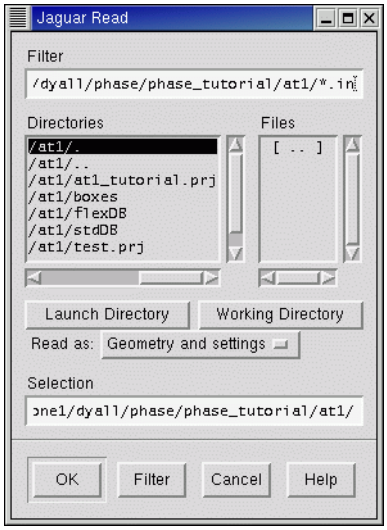


Figure 2.2. The Jaguar Read File ***file selector.***

For example, if you imported three conformers of decane from a file in which each conformer had the name `decane`, the entry names would be `decane-imp1.1`, `decane-imp1.2`, and `decane-imp1.3`.

The same naming mechanism is used when calculation results are incorporated into a project, except that the suffix `-inc`*j* is added to the entry name.

2.1.5 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 Jaguar from the Applications menu, then click Read in the Jaguar panel. The Read File 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*.

2.2 Exporting Structures

Using the Export panel, you can write out structure files in Maestro, MacroModel, PDB, Sybyl Mol2, and MDL SD 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 panel, choose Export Structures from the Project menu on the main menu bar, or choose Structures from the Export submenu of the Table menu in the Project Table panel.

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.

2.2.1 Selecting Export Settings

The Export panel is laid out in a similar fashion to the Import panel, with the file and file type selection tools at the top, and various options under them.

Selecting a file format: To create a file, you must select the type of file you wish to write from the types given in the Format option menu, which include Maestro, MMOD (MacroModel), PDB, Mol2, SD, and a range of file types converted by Babel. The file extension in most cases is determined by the file type. Default file extensions for the files in the first section of the menu can be set in the File Suffix folder of 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.

Selecting a directory: To select a directory, you can enter it in the Path text box, navigate to it in the Directories list, or click Launch Directory or Current Directory to select the directory from which you launched Maestro or the current working directory. The path and the directory and file lists are updated for the chosen directory.

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

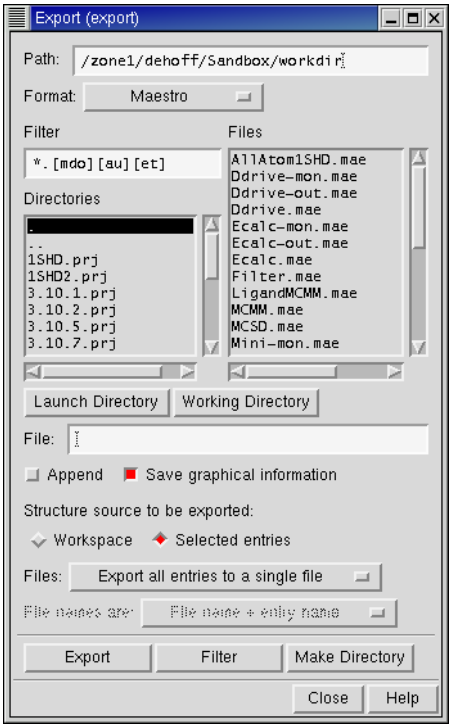


Figure 2.3. The Export ***panel.***

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.

Saving graphical information: If you are writing a Maestro file, you can select Save Graphical Information to store the molecular representation information for the structure you are saving. This option is ignored for other file types.

Specifying the source of the structures: The Export panel can be used to save structures directly from the Workspace or to write files containing structures associated with one or more project entries. To write out the Workspace to a file, select Workspace in the Structure Source To Be Exported section. This is equivalent to writing the included entries. To write out the entries that are selected in the Project Table to the exported file, select Selected Entries.

Exporting to single or multiple files: You can export entries to a single, multi-structure file, or to multiple files that each contain a single entry. From the Files option menu, choose either Export All Entries To A Single File or Export Each Entry As An Individual File. If you export structures using one of the Babel-supported formats, you can only export a single structure to each file. In this case, you should not choose Export All Entries To A Single File.

2.2.2 Exporting Multiple Files

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

File Name + Entry Name

If you choose File Name + Entry Name, you must select a file or type in a file stem. The entry name 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` in Maestro format, and you select the file `structure.dat`, the new files are named

```
structure_combination-3.dat
structure_combination-4.dat
structure_combination-5.dat
```

If you typed in the file stem `HIV`, the following files would be written:

```
HIV_combination-3.mae
HIV_combination-4.mae
HIV_combination-5.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 same example as above, if you select the file `structure.dat`, the new files are named

```
structure_1.dat
structure_2.dat
structure_3.dat
```

Just Entry Names

If you choose Just Entry Names, the file name is constructed from the entry name. 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.

2.3 Exporting Data to a Spreadsheet

The Project Table does not have 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 Show Table from the Project menu in the main window or clicking the Show/Close project table button in the toolbar.

When the Project Table panel is displayed, choose Spreadsheet from the Export submenu of the Table menu. The Export Spreadsheet panel is displayed. The layout of this panel is similar to that of the Export and Import panels, with file selection tools at the top and action buttons at the bottom.

Selecting a directory: To select a directory, you can enter it in the Path text box, navigate to it in the Directories list, or click Launch Directory or Current Directory to select the directory from which you launched Maestro or the current working directory. The path and the directory and file lists are updated for the chosen directory.

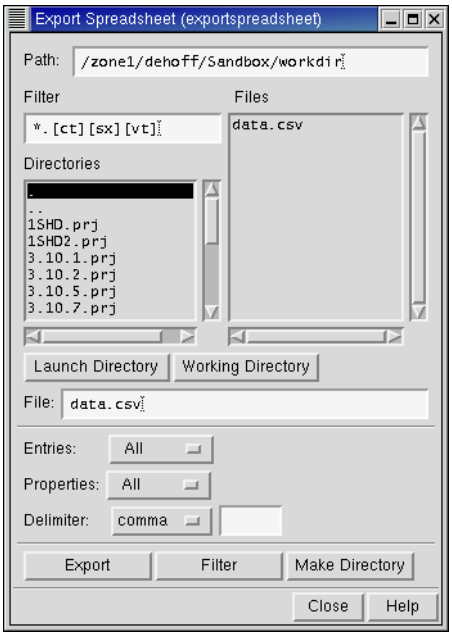


Figure 2.4. The Export Spreadsheet ***panel.***

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

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. For more information on showing, selecting, and including entries, see Section 7.4 on page 92 and Section 7.5 on page 95.

Selecting properties to export: You can choose to export all properties or only the shown properties, using the Properties option menu. The row number and the inclusion state are not exported, but all other properties are. The entry name is always in the first column.

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 Export. The file is written and its name is displayed in the Files list.

2.4 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 panel, 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 Show/Close project table button in the toolbar.

When the Project Table panel is displayed, choose Spreadsheet from the Import submenu of the Table menu. The Import Spreadsheet panel is displayed. The layout of this panel is similar to that of the Export and Import panels, with file selection tools at the top and action buttons at the bottom.

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 text box.

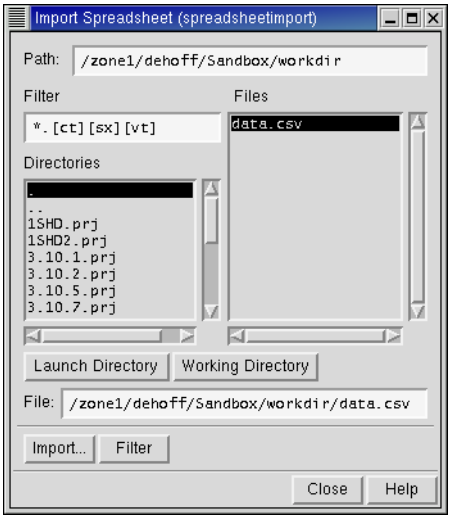


Figure 2.5. The Import Spreadsheet ***panel.***

When you have selected the file, click Import. The Choose Import Key dialog box is displayed. 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. 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.

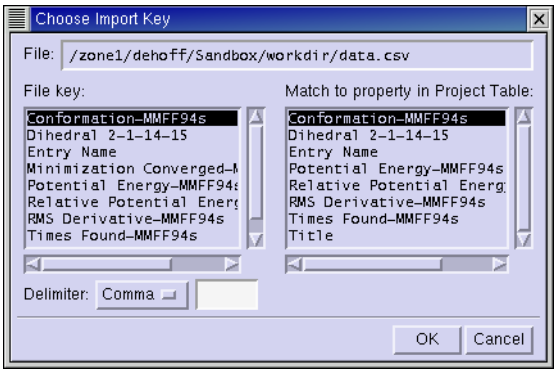


Figure 2.6. The Choose Import Key ***dialog box.***

To complete the import, choose the delimiter that is used in the spreadsheet file, then click OK. The values in the spreadsheet are imported into the Project Table.

Building Structures

Maestro provides a variety of tools for building and modifying structures. In the Build panel, you can create molecular structures from predefined fragments or from individual atoms, and modify structures and atom and residue properties. 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 4.

3.1 The Build Panel

The Build panel consists of a toolbar and three tabbed folders. The primary building tools are contained in the Fragments folder and the toolbar. The Fragments folder 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 folders, Atom Properties and Residue Properties, contain tools for changing the properties of atoms or residues.

To open the Build panel, choose Build from the Edit menu, or click the Open/Close Build panel button on the main toolbar.

The Fragments folder is displayed by default.

The toolbar of the Build panel provides quick access to tools for drawing and modifying structures and labeling atoms. See Section 1.3.2 on page 7 for a description of the types of toolbar buttons. The toolbar buttons are described below, and their use is described later.

Draw
Choose an element for drawing structures freehand in the Workspace (default C). Each click in the Workspace places an atom and connects it to the previous atom.

Delete
Choose an object for deleting. Same as the Delete button on the main toolbar, see page 8.

Set element
Choose an element for changing atoms in the Workspace (default C). Click an atom to change it to the selected element.

Increment bond order
Select a bond to increase its bond order by one, to a maximum of 3.

Decrement bond order
Select a bond to decrease its bond order by one, to a minimum of 0.

Increment formal charge
Select an atom to increase its formal charge by one.

Decrement formal charge
Select an atom to decrease its formal charge by one.

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.

Label
Apply heteroatom labels as you build a structure. The label consists of the element name and formal charge, and is applied to atoms other than C and H.

Display Connect/Fuse panel
Open the Connect & Fuse panel so you can connect structures (create bonds between structures) or fuse structures (replace atoms of one structure with those of another).

Display Adjust panel
Open the Adjust panel so you can change bond lengths, bond angles, dihedral angles, or atom chiralities.

Add hydrogens
Choose an atom type for applying the current hydrogen treatment. Same as the Add hydrogens button on the main toolbar, see page 9.

Geometry Symmetrizer
Open the Geometry Symmetrizer panel for symmetrizing the geometry of the structure in the Workspace.

Geometry Cleanup
Cleans up the geometry of the structure in the Workspace.

3.2 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. The following fragment libraries are available with Maestro:

- 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
- Protein capping groups
- Deoxyribonucleic acids
- Ribonucleic acids
- Double-stranded A DNA
- Double-stranded B DNA
- Double-stranded A RNA
- Double-stranded B RNA

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, using the Elements menu option in the Atom Properties folder.

- **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.
- **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.
- **Protein capping groups**—This library contains some common molecules used to cap peptides.

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 folder.

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 to obtain the appropriate instructions.

3.2.1 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. To enter Place mode, select Place in the Fragments folder.

To create multiple structures in the Workspace in Place mode, choose a library from the Fragments option menu, select a fragment, and 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 want to join these structures to form a single molecule, you can use the tools in the Connect/Fuse panel. See Section 3.6 on page 40 for details.

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 from the fragments list and clicking in the Workspace on the atom that you want the new fragment to

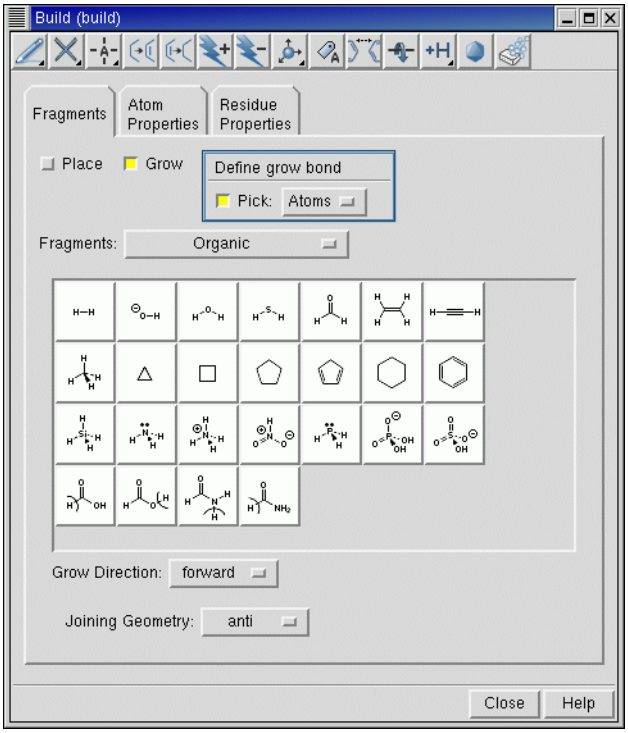


Figure 3.1. The Fragments ***folder of the*** Build ***panel, showing the*** Organic ***library.***

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.

You can also mutate one residue into another in a protein. When you select Amino acids from the Fragments menu, 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.

3.2.2 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 folder.

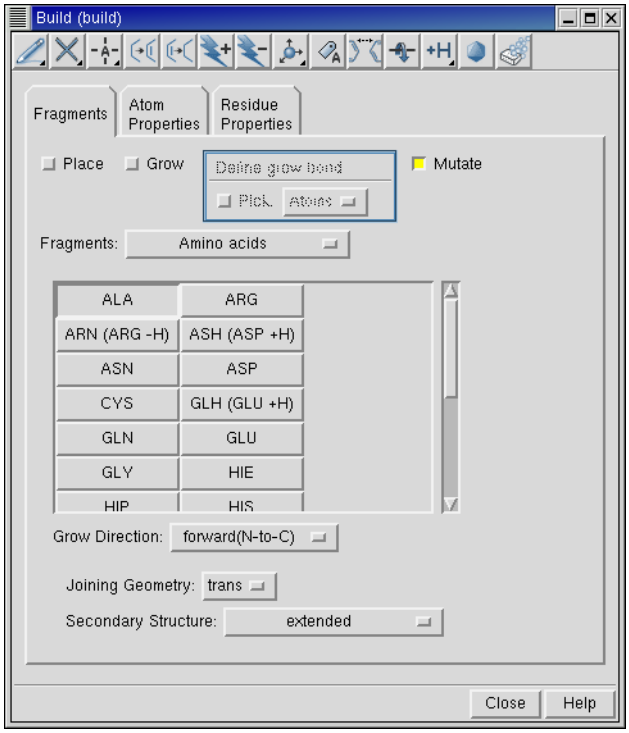


Figure 3.2. The Fragments ***folder of the*** Build ***panel, showing the*** Mutate ***option.***

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 folder 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 an angle value is displayed. Enter a value and click OK.

3.3 Building a Structure From Atoms

The toolbar of the Build panel contains tools for drawing structures in the Workspace atom by atom, and the Atom Properties folder 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 molecular structure, only a few elements—H, C, N, O, P, and S—are available. If you want to include different elements, use these elements to draw the structure, and then change the desired atoms—see Section 3.4. 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 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 indicates that the atom is active, which means that it will be automatically connected 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.
- 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, select the element from the Draw button menu. 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 x-y plane. 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 x-y 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.

3.4 Changing Elements

Whether you build a molecule in Place mode, Grow mode, or Draw mode, the range of elements available to you is limited. To include other elements in your structure, you must first build with existing elements, then change the element to another element in the appropriate locations in the structure. 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 panel toolbar or from the Atom Properties folder. From the Set Element button menu in the toolbar

you can choose an element from H, C, N, O, P, or S, then click on an atom in the Workspace to change it to the selected element.

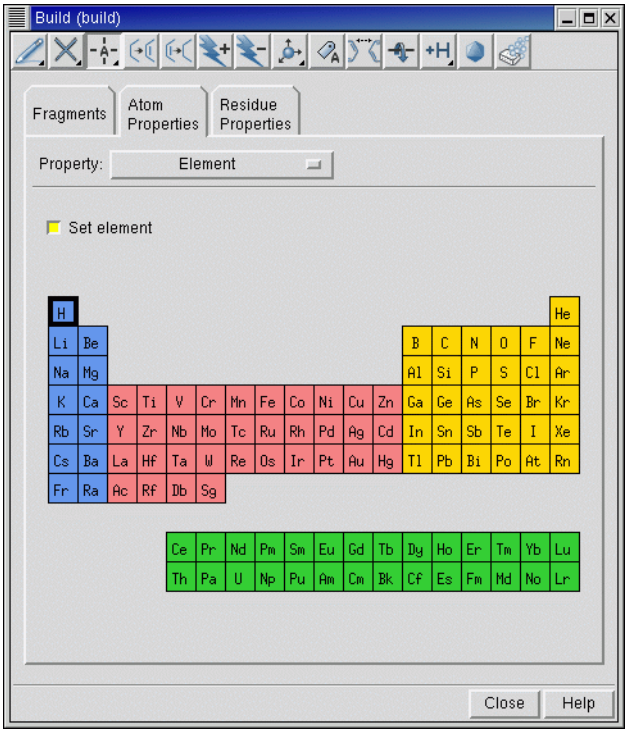


Figure 3.3. The Atom Properties ***folder showing tools for the*** Element ***property.***

If you want to change an atom to some other element, choose Element from the Property menu in the Atom Properties folder. 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. However, you can select Set Element if it is unselected and you want to use the currently selected element.

3.5 Changing the Bond Order and Formal Charge

After creating a structure using the tools in the Build panel, you may wish to change some of the bond orders or formal charges. You can make these changes with the tools on the Build panel toolbar (as shown below) or by right-clicking a bond and choosing the appropriate item from the shortcut menu[1].

1. By default, right-clicking with the mouse displays a context-sensitive shortcut menu. You can turn off this option by choosing Preferences from the Maestro menu and selecting the appropriate option in the Mouse folder.

- To increase the bond order, click the Increment 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 Decrement 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 a green line.

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 Increment formal charge 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 Decrement formal charge 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.

3.6 Fusing or Connecting 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.

The tools for fusing and connecting structures are available from the Connect & Fuse panel. 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 atom selected first replaced by the second selected atom. 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.

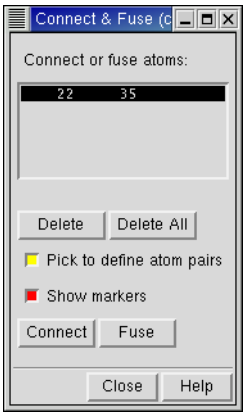


Figure 3.4. The Connect & Fuse ***panel.***

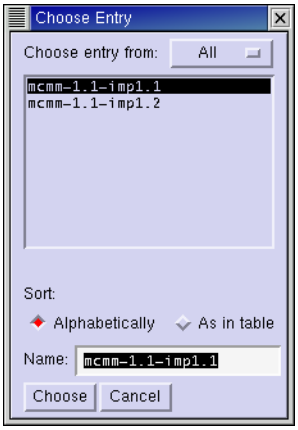


Figure 3.5. The Choose Entry ***dialog box.***

To delete an atom pair from the Connect or Fuse Atoms list and cancel the connection or fusion of those atoms, 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 is displayed, 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.

  The Choose Entry dialog box provides some tools for selecting the destination entry: a menu to limit the entries listed, and some sort options.
- If you provide a new entry name in the Name text box, the source entries are deleted, and a new entry is created that contains the fused or connected structure.

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

3.7 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.

3.7.1 Adjusting Parameters

In addition to the adjustments you can make with the Move button, described on page 32, you can also change bond lengths, bond angles, dihedral angles, and atom chirality. You can make these adjustments either in the Workspace directly or by using the tools in the Adjust panel.

In the Workspace

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

1. Click the Adjust distances, angles or dihedrals button in the main toolbar:

   and choose Distance.

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

   The bond 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 middle mouse button, click on the defined bond and drag to the right to lengthen the bond or to the left to shorten it.

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

From the Adjust Panel

You can open the Adjust panel from the Edit menu in the main window, or with the Display Adjust panel button on the Build panel toolbar.

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 folder and select dihedrals by the residues in each entry (or chain), or by standard names.

The atom numbers of the selected atoms are listed in the table in the center of the folder. You can pick as many sets of atoms as you like before doing any adjustments. The last atom that you pick is the "target atom"—the atom that is moved in the adjustment process.

Once you have chosen the atoms, you must 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.

To make the adjustment, you can enter a new value for the geometric parameter in the text box, or you can use the mouse. If you enter a new value, the value is changed and the Workspace updated when you press ENTER. To adjust the geometry using the mouse, select Allow adjusting then drag with the middle mouse button to adjust the geometry.

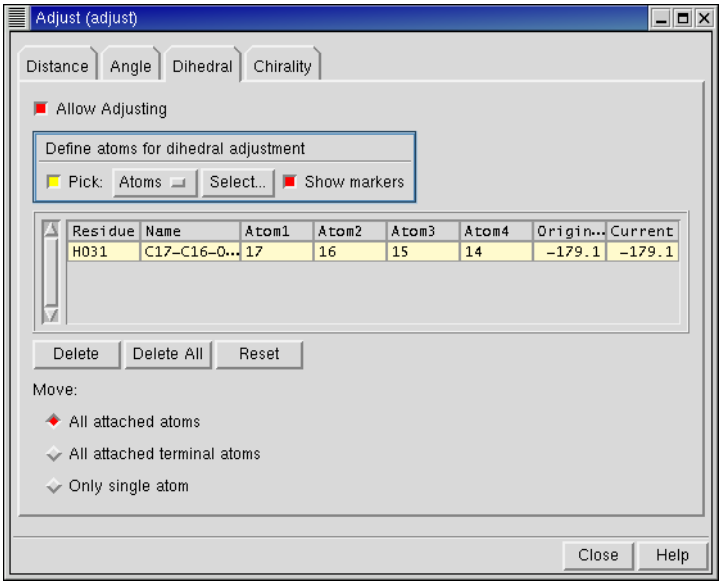


Figure 3.6. The Adjust ***panel, showing the*** Dihedral ***folder.***

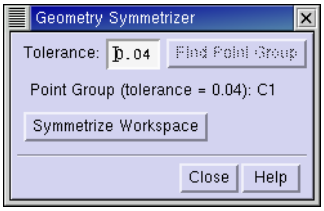


Figure 3.7. The Geometry Symmetrizer ***panel.***

To adjust the stereochemistry at a chiral center, use the picking tools in the Chirality folder. You can invert the chirality of selected chiral centers or of all chiral centers. This folder 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.

3.7.2 Cleaning up the Geometry

Geometry Symmetrizer

The Geometry Symmetrizer allows you to symmetrize the geometry of the structure in the Workspace, subject to a given tolerance.

To use the Geometry Symmetrizer:

1. Choose Symmetrize from the Edit menu, or click the Geometry Symmetrizer toolbar button in the Build panel.

2. Click Find Point Group and check to see whether the desired point group is found for the structure in the Workspace. If not, increase the tolerance and click Find Point Group again.
3. When the desired point group is found, click Symmetrize Workspace.

Geometry Cleanup

To clean up the structure in the Workspace, the Geometry Cleanup utility minimizes the energy of the structure using a Universal Force Field (UFF). It realigns atoms that are too crowded and corrects unphysical geometry that can occur when building molecules from the Build panel. In general, it eliminates distortions that can cause jobs to fail (for instance, MacroModel or Jaguar jobs).

To run Geometry Cleanup, choose Cleanup from the Edit menu, or click the Geometry Cleanup toolbar button in the Build panel.

Note: Geometry Cleanup only works for structures with less than 300 atoms, and can be slow for structures with more than 200 atoms.

3.8 Applying a Hydrogen Treatment

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 and 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 Hydrogen Treatment panel, which you open from the Edit menu.

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 3.1.

Table 3.1. Appropriate hydrogen treatments for Maestro-supported force fields

Hydrogen Treatment Method	MM3	MM2	AMBER	AMBER94	MMFF	MMFFS	OPLS-AA, OPLS2001	OPLS
All-atom with No-Lp	X	X		X	X	X	X	
All-atom with Osp3-Lp		X						
Csp3 United-atom with S-Lp[a]			X					
Csp3 United-atom with No-Lp[a]								X
All atom with S-Lp			X					
Csp2/sp3 United atom with No-Lp[a]								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.

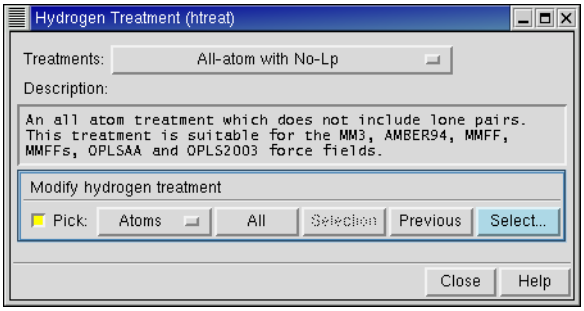


Figure 3.8. The Hydrogen Treatment ***panel.***

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 click Apply Current Treatment To All Atoms.

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 entities from the Add hydrogens button menu,

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

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.

3.9 Changing Atom Properties

In addition to changing the element and the formal charge, you can change a variety of other atom and residue properties. The tools for making changes are in the Atom Properties folder. 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. Before you change atom properties, it may be helpful to display atom labels. For atom labeling information, see Section 5.3 on page 72.

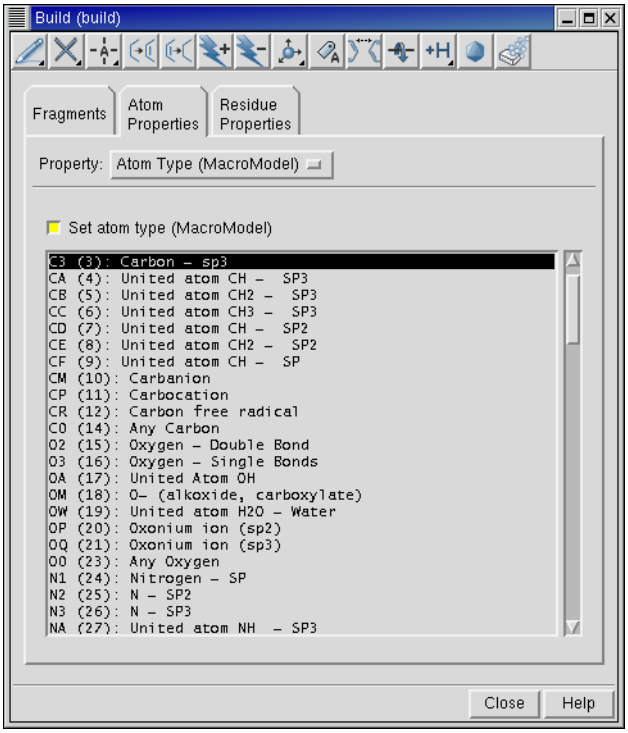


Figure 3.9. The Atom Type (MacroModel) ***tools in the*** Atom Properties ***folder.***

Atom type (MacroModel)

A list of atom type symbols with a brief description is displayed (see Figure 3.9). 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. 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. To retype an atom, choose the atom type and click on the atoms in the Workspace that you want to change.

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.

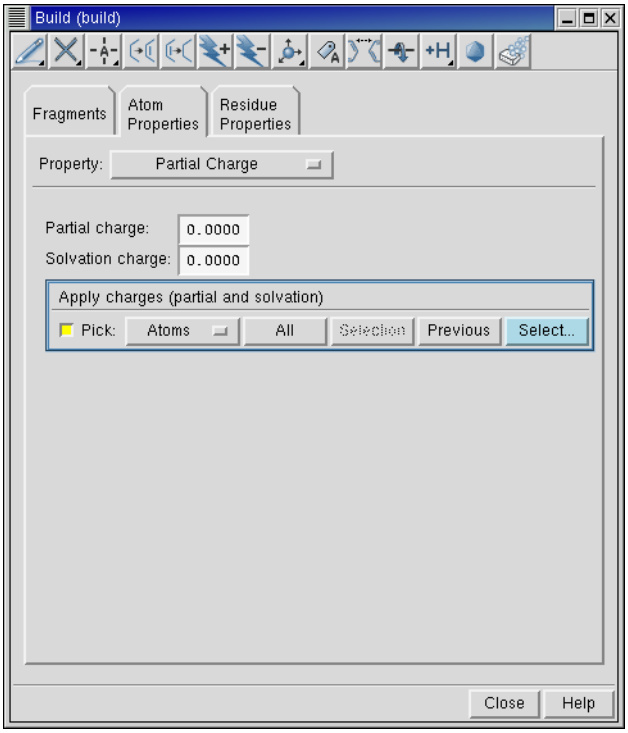


Figure 3.10. The Partial Charge ***tools in the*** Atom Properties ***folder.***

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, when reading or writing a PDB file, 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

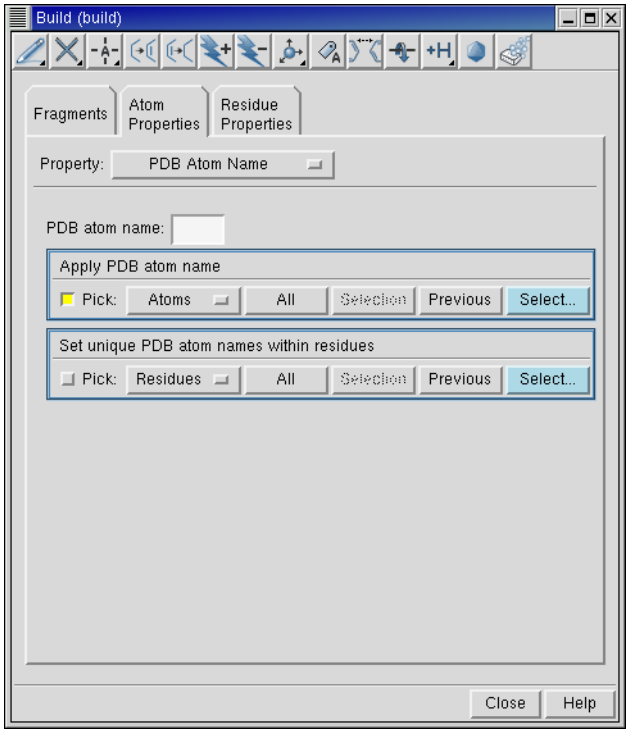


Figure 3.11. The PDB Atom Name ***tools in the*** Atom Properties ***folder.***

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.

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.

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 desired 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,

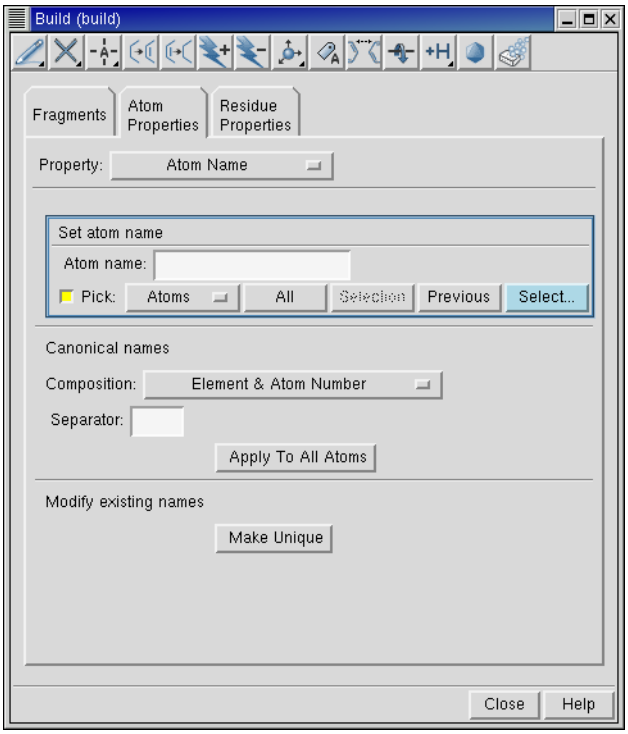


Figure 3.12. The Atom Name ***tools in the*** Atom Properties ***folder.***

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.

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.

3.10 Changing Residue Properties

Residue properties can be changed in the Residue Properties folder. This folder is laid out in a similar fashion to the Atom Properties folder, 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 residues, in 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. Renumbering a single residue is the same as assigning its number. To apply a specific 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.

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.

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,

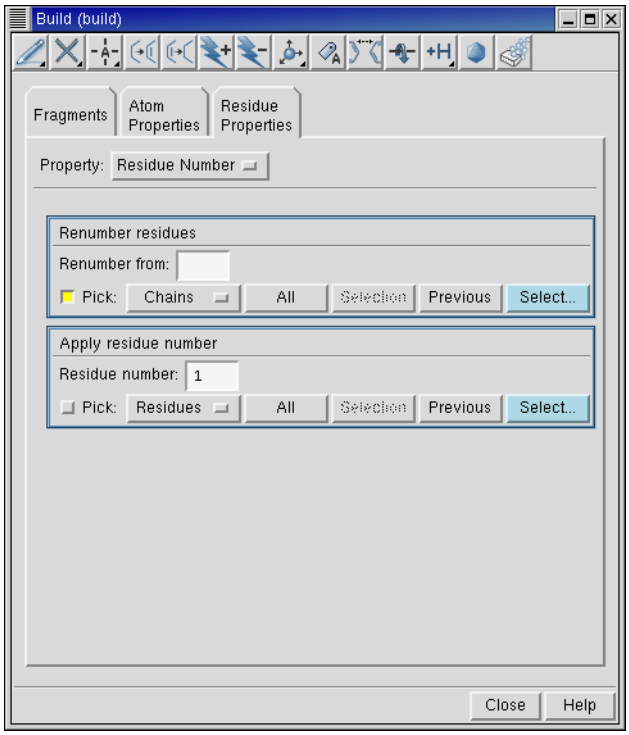


Figure 3.13. The Residue Number ***tools in the*** Residue Properties ***folder.***

and assign it a name. To assign the name, enter a character in the Chain Name text box and use the picking tools to define the chain.

3.11 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. To define a centroid, select Pick atoms to define centroid, pick the atoms in the Workspace. The atoms are listed in the Atoms to define centroid list. If you have Show 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. The To define another centroid, click Delete All before picking atoms for the new centroid.

3.12 Deleting Atoms

If you need to delete atoms from a structure, you can use the Delete button menu on either the main toolbar or the Build panel toolbar.

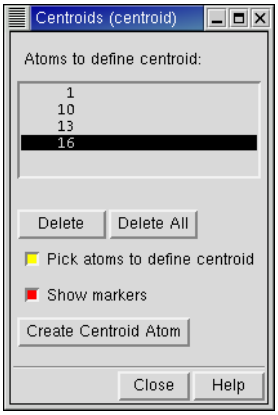


Figure 3.14. The Centroids ***panel.***

This menu offers choices for the type of object to delete, and allows you to open the Atom Selection dialog box to select atoms for deletion based on their properties.

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 folder of the Preferences panel.

If you want to delete all atoms in the Workspace, use the Clear Workspace button, which is located on the main toolbar.

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

4.1 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 an object type 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 Workspace selection button:

1. Choose Residues from the Workspace selection toolbar button:

   The button changes to:

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

   You can also drag to select multiple residues.

4.2 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 an object type for selecting. The Pick Option Menu is described on page 56.
- All button—Performs the action on all atoms in the Workspace.

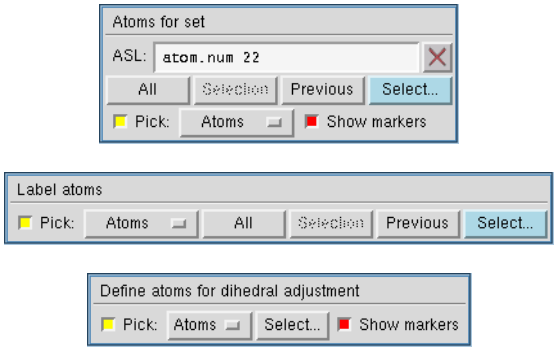


Figure 4.1. Examples of picking tools. Top: from the Sets ***panel; Center: from the*** Atom Labels ***panel; Bottom: from the*** Adjust ***panel.***

- Selection button—Performs the action on any atoms already selected in the Workspace.
- Previous button—Performs the action on the most recent atom selection defined in the Atom Selection dialog box (see Section 4.3 on page 57).
- Select button—Opens the Atom Selection dialog box (see Section 4.3 on page 57).
- ASL text box—Allows you to type in an ASL expression for selecting atoms.

  ASL stands for Atom Specification Language, and is described in detail in the *Maestro Command Reference Manual*.
- Clear button—Clears the current selection.

- Show markers option—Marks the selected atoms in the Workspace

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 Label Atoms section of the Atom Labels panel has a Pick option menu, an All button and a Select 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.

The Pick Option Menu

With the Pick option menu, you can choose an object type (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

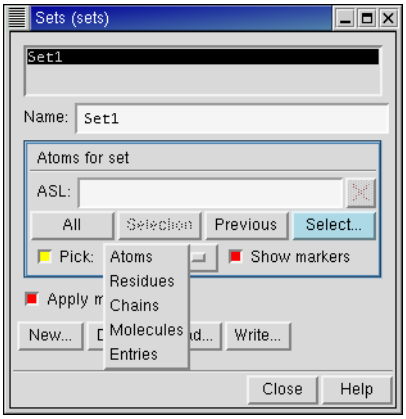


Figure 4.2. The* Sets *panel, showing the* Pick *option menu.

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 an object type, 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.

The number of object types 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.

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

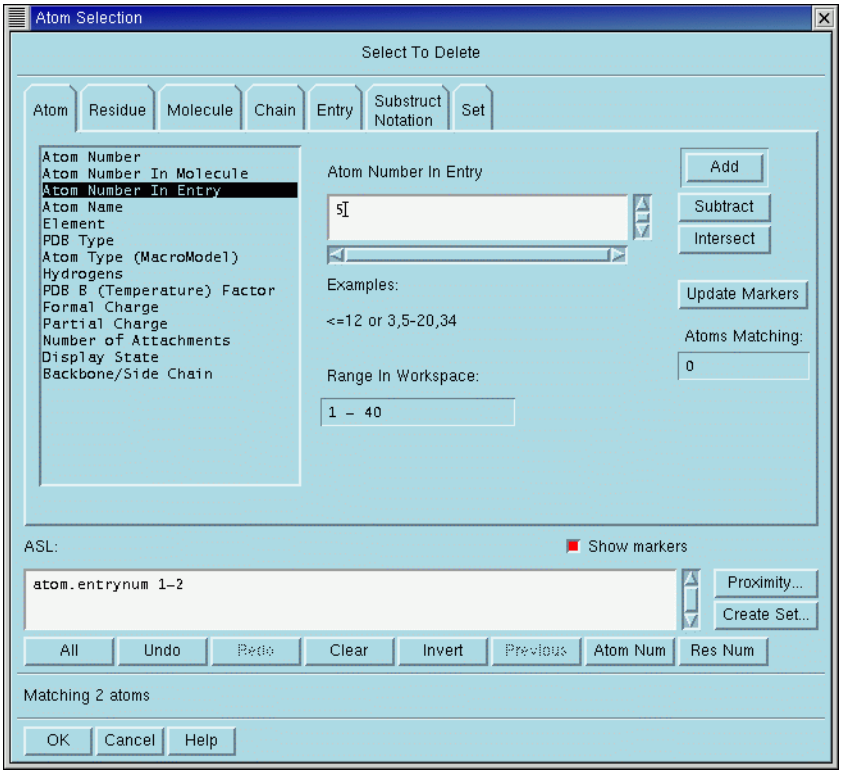


Figure 4.3. The** Atom Selection **dialog box.

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 (see Section 4.2 on page 55).

To select atoms

1. Create an atom group by selecting a property and value (see Section 4.3.1 on page 59).
2. Click Add or Subtract to define the current selection (see Section 4.3.2 on page 59).
3. Create more atom groups as needed and click Add, Subtract, or Intersect to modify the current selection (see Section 4.3.2 on page 59).
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.

4.3.1 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 folder: Atom, Residue, Molecule, Chain, Entry, Substructure Notation and Set. For each category there is a list of properties shown on the left of the folder, from which you can select one item. When you select an item, tools for that property are displayed in the center of the folder. 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. >= 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.

4.3.2 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
- Undo—undo the last operation
- Red—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
- 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.

4.3.3 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 4.4 on page 60. 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. You can either include or exclude the source atoms in the

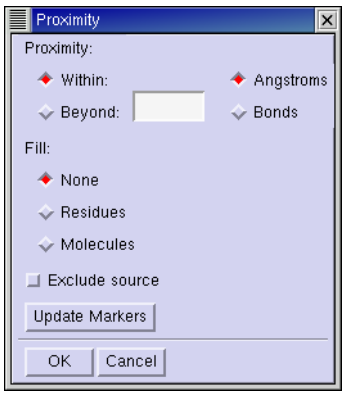


Figure 4.4. The Proximity ***dialog box.***

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.

4.3.4 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 folder. 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 8.4 on page 116.

4.3.5 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 folder, 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.
7. 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 folder, 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 folder, 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 folder, 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.

Displaying 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.

5.1 Changing Atom Color

Changing the color of a structure can help you to visualize its properties and its three dimensional structure. The Atom Coloring panel controls allow you to apply a new color to all or some of the Workspace atoms, 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.

To open the Atom Coloring panel, choose Atom Coloring from the Display menu.

5.1.1 Applying a Single Color

To apply a single color scheme to some or all atoms in the Workspace, you can use the tools in the Atom Color folder. This folder contains a color palette in the By Palette subfolder (see Figure 5.1 on page 64), and a list of color names in the By Name subfolder Figure 5.2 on page 64). You can use either of these to select a color. Once you have selected a color, use the picking tools in the subfolder to apply the color to selected atoms, or click the All button to apply the color to all atoms in the Workspace.

You can also apply a color from the Color residues by constant color button menu in the 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 folder to select the color.

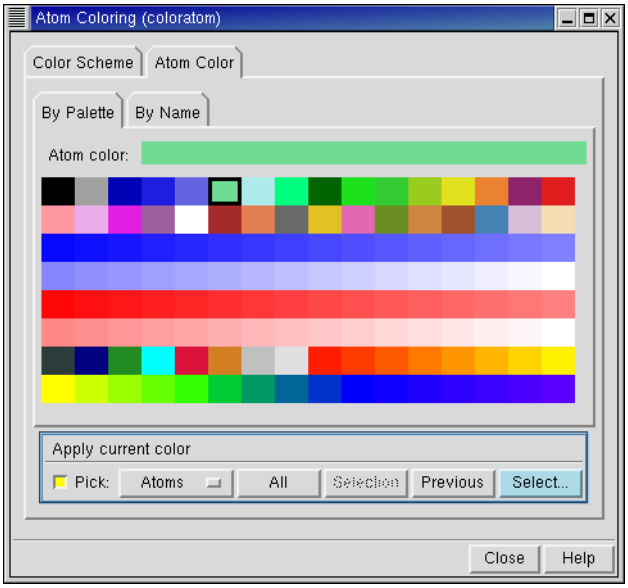


Figure 5.1. The By Palette ***folder of the*** Atom Coloring ***panel.***

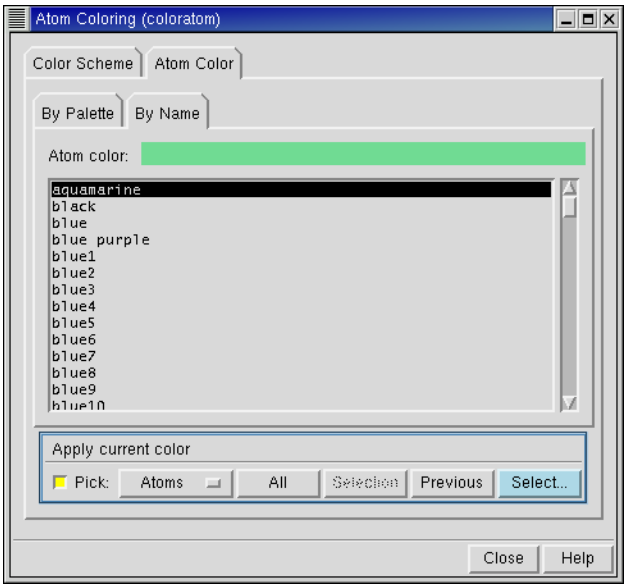


Figure 5.2. The By Name ***folder of the*** Atom Coloring ***panel.***

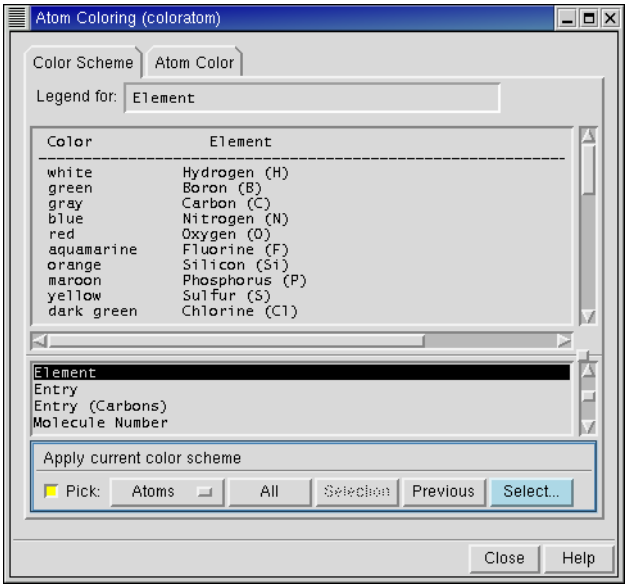


Figure 5.3. The Color Scheme ***folder of the*** Atom Coloring ***panel.***

5.1.2 Using Predefined Schemes to Color Atoms

To apply coloring to some or all Workspace atoms using one of Maestro's predefined color schemes, you can use the tools in the Color Scheme folder (see Figure 5.3). Click on the desired scheme name in the list in the lower portion of the panel. The legend at the top of the panel describes the colors that will be applied and the criteria used to apply them. Once you have selected a scheme, use the picking tools to select the atoms you wish to color, or click the All button to apply the selected color scheme to all atoms in the Workspace.

You can also 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 color scheme is applied when you make your menu choice. The schemes are described in the Color Scheme folder.

5.2 Changing Molecular Representations

The Molecular Representation panel contains four folders, Settings, Atoms, Bonds, and Ribbons. The Ribbons folder contains controls for representing the structure of proteins.The first three folders contain controls for setting molecular representation for the atoms and bonds in the Workspace and for setting the molecular representation in which subsequently drawn atoms and bonds are displayed. Using the controls in these folders, you can choose to change the molecular representation for all atoms and bonds in the Workspace, for only the atoms currently in the Workspace, or for only the bonds currently in the Workspace. You can also use the shortcuts available in the toolbar to change the molecular representation.

To open the Molecular Representation panel, choose Molecular Representation from the Display menu.

5.2.1 Changing the Representation of Atoms

In the Atoms folder, you can choose between None, CPK and Ball & Stick for the representation of atoms. The None option means that only the bonds are depicted. The bond representation is set in the Bonds folder. To change the representation of the atoms, use the picking tools or the Select button in the Apply current representation to atoms section to select atoms to apply the

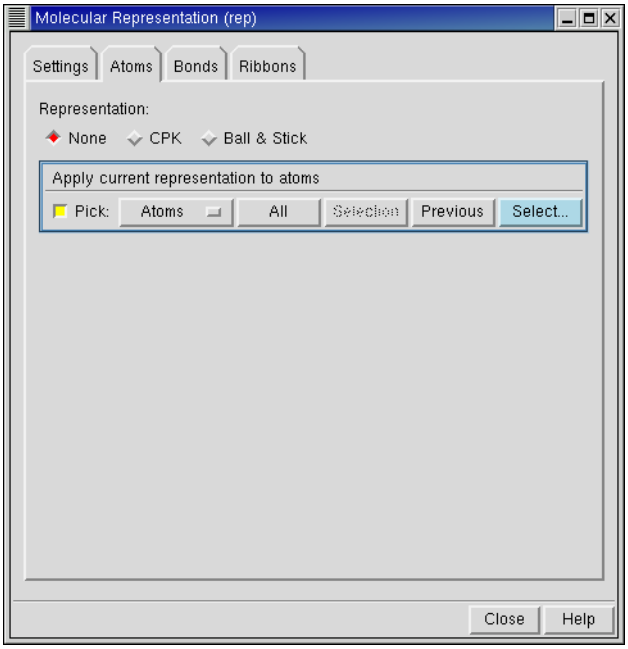


Figure 5.4. The Atoms ***folder of the*** Molecular Representation ***panel.***

representation, or click All to apply the representation to all atoms. You can mix representations within a single molecule by picking.

The Ball & Stick option sets a representation for both atoms and bonds. When you pick an individual atom in this representation, half of each bond attached to the picked atom is displayed in stick form.

You can apply a molecular representation using the Draw atoms in CPK representation and Draw atoms in Ball & Stick representation buttons on the toolbar. Click either button to pick the objects to apply the representation to. Double-click either button to apply the representation to all atoms. You can choose the object to pick from the button menus.

5.2.2 Changing the Representation of Bonds

In the Bonds folder you can choose between None, Wire, and Tube for the representation of bonds. The None option means that only the atoms are displayed. To change the bond representation for selected atoms, use the picking tools or the Select button in the Apply current representation to atoms section. Click All to apply the representation to all bonds. You can mix representations within a single molecule by picking.

If you choose the Wire representation, several other options are also available in the Wire Settings section:

- Style: You can select Split to display distinctly colored half-bonds, or Blend to display bonds as color gradients. Selecting Blend can improve graphics performance.
- Represent bond orders with: You can choose Multiple Lines to display multiple bonds as multiple lines, or Thickness to display multiple bonds as thicker lines, as in earlier versions of Maestro.
- Show Bond Orders: You can choose when to display multiple bonds. Automatically means that bond orders are displayed at high zoom but are not displayed at low zoom. The threshold for the display of bond orders can be changed with the Maestro command `repall borderscale=`*value*. The default for *value* is 30 Å, and represents the width of the portion of the structure visible in the Workspace.
- Smoothing: You can smooth the lines that represent bonds. Smoothing Wire bonds especially enhances the viewing of larger structures. However, smoothing can prevent multiple bonds from being displayed correctly in the Thickness representation. If you do not see thick bonds, deselect this option.

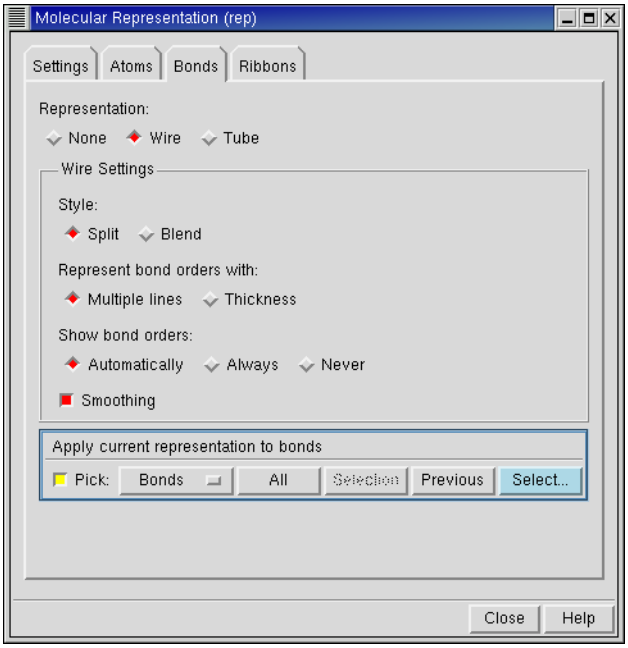


Figure 5.5. The Bonds ***folder of the*** Molecular Representation ***panel.***

To apply the new representation, use the picking tools or the Select button to select bonds, or click All to select all bonds.

You can also apply a molecular representation using the Draw bonds in wire and Draw bonds in tube buttons in the toolbar.

Click either of these buttons to pick the object to apply the representation to. Double-click either button to apply the representation to all atoms. You can choose the object to pick from the button menus.

5.2.3 Changing Representation Attributes

The controls in the Settings folder allow you to customize the appearance of the Wire, CPK, Tube, and Ball & Stick representations. It also provides a quick means of applying a representation to all atoms to view the changes made.

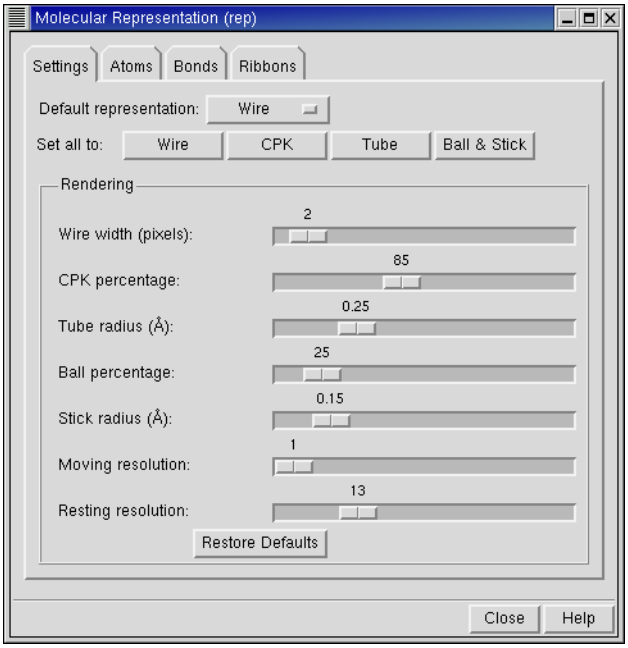


Figure 5.6. The Settings ***folder of the*** Molecular Representation ***panel.***

To change the default representation, so that any subsequently placed atoms use the new representation, select a representation from the Default Representation to menu at the top of the folder. Changing the default representation does not affect the representation of any atoms or bonds currently in the Workspace.

You can adjust the parameters of the representations using the sliders in the Rendering section and apply the representation using the buttons. If the representation is already selected, changes made using the sliders take effect immediately.

The seven slider controls have the following functions:

- Wire Width (pixels)—adjust the width of the lines used to represent bonds in the Wire representation.
- CPK Percentage—change the volume of the spheres in CPK mode as a percentage of the van der Waals radius.
- Tube Radius (Å)—change the radius of the tubes in Tube mode.
- Ball Percentage—change the volume of the spheres in Ball & Stick mode as a percentage of the van der Waals radius.
- Stick Radius (Å)—change the radius of the sticks in Ball & Stick mode.

- Moving Resolution—change the resolution of the ball rendering during translation and rotation. A low resolution can speed up translations and rotations.
- Resting Resolution—change the resolution of the ball rendering when the structure is not being moved.

5.2.4 Rendering Proteins as Ribbons

The controls in the Ribbons folder enable you to display protein backbones as a ribbon diagram. Displaying ribbons can simplify the analysis of the protein's 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.

You can open the Molecular Representation panel with the Ribbons tab displayed by choosing Ribbons from the Display menu 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.

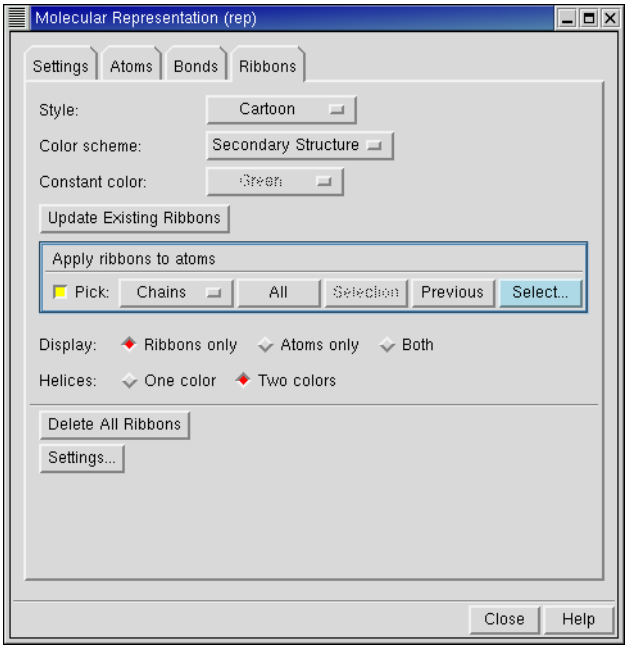


Figure 5.7. The Ribbons ***folder of the*** Molecular Representation ***panel.***

- Tube—curved tube that follows the backbone.
- Thin Tube—thin curved tube that follows the backbone.
- Curved Line—curved line that follows the backbone.
- CA Trace—straight line that connects alpha carbon atoms.
- CA Trace Tube—straight tube that connects alpha carbon atoms.

With the exception of the CA Atom Color scheme, the color schemes are described in the Color Scheme folder of the Atom Coloring panel. 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. You can also select a two-color representation of helices, using the Helices options in the lower part of the panel. The chosen color scheme is applied to the outside of the helix, and the inside of the helix is gray.

To apply the chosen style and color scheme, you can use the picking tools in the Apply Ribbons To Atoms section, or click Select to use the Atom Selection dialog box, or click All. You can apply the current scheme to all existing ribbons by clicking Update Existing Ribbons. If you want to change the scheme for a part of the protein or for one existing ribbon rather than all ribbons, use the tools in the Apply Ribbons to Atoms section.

The display options in the lower part of the folder allow you to display the ribbons only, the atoms only, or both. The atom display operates only on the already displayed atoms, and only on the atoms for which a ribbon is defined.

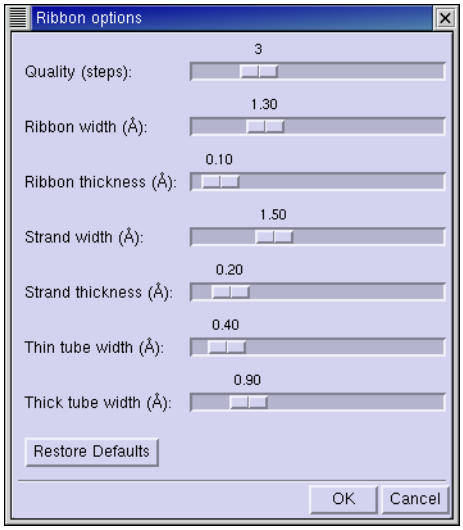


Figure 5.8. The Ribbon options ***dialog box.***

You can apply the color schemes and the display options using the Show, hide, or color ribbons toolbar button menu.

If you want to change the quality of the ribbons, or the width or thickness of the ribbons, strands, or tubes, click Settings. The Ribbon options dialog box is displayed. This dialog box has slider controls for quality, ribbon width, ribbon thickness, strand width, strand thickness, thin tube width, and thick tube width, and a button to restore the default values.

5.3 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.

To open the Atom Labels panel, choose Atoms Labels from the Display menu.

Options for labeling atoms with a variety of atom, molecule, residue, chain, and entry properties are provided in the Composition folder of the Atom Labels panel. To compose a label, select as many properties as you like. The properties are separated by spaces in the label. If you select User Text, you can enter text in the text box to include your own information in the labels.

The color of the labels is the color of the labeled atom, by default. To use a fixed color for the label, deselect Color label by atom in the Color folder, and select a color in the By Palette or By Name subfolder. These subfolders are identical to those in the Atom Coloring panel.

Instead of choosing your own labels, you can choose from two fixed labeling schemes that label non-carbon atoms with the element name. In the Hetatom Labels folder, you can select Labels on hetero and hydrogen atoms to label all non-carbon atoms with the element label, or Labels on hetero atoms to label all atoms other than carbon and hydrogen with the element label. When you select either of these schemes, the labels are applied immediately to all relevant atoms. The Labels on hetero atoms scheme is also available from the Build panel toolbar, and is applied as atoms are added to the Workspace.

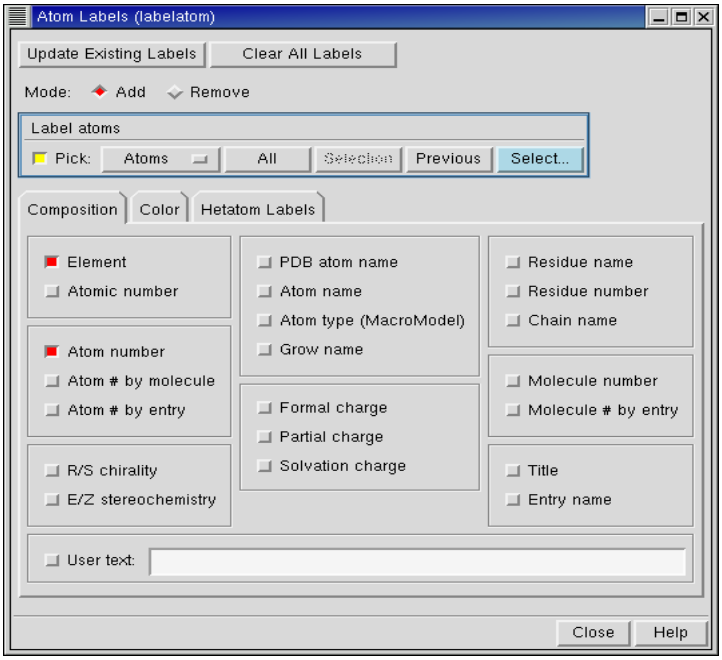


Figure 5.9. The Atom Labels ***panel.***

To select the atoms for labeling, use the tools in the Label atoms section. You can use the picking tools, click All to label all atoms, or click Select and use the Atom Selection dialog box to choose the atoms to label. When you modify the label contents or appearance, you can update all labels with the new definitions by clicking Update Existing Labels.

If you want to remove some or all labels, select Remove in the Mode section. The Label atoms section is relabeled Clear Labels. Use the tools in this section to remove labels. When you select Remove, the label composition is no longer relevant.

You can also label atoms from the toolbar. To apply a single property from a subset of the full range of properties to all atoms, use the Label Atoms button menu:

To apply the current labeling scheme by picking, use the Label Picked Atoms 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 folder 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.

If you want to customize the appearance and position of the label, you can do so in the Label folder of the Preferences panel. See Section 11.2.4 on page 147 for information.

5.4 Displaying and Undisplaying Atoms

The Display/Undisplay Atoms panel allows 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, sidechains, water molecules, or hydrogen atoms. If you want to display and undisplay project entries, use the In setting in the Project Table panel. See Section 7.5.1 on page 95 for more information about operating on project entries.

To open the Display/Undisplay Atoms panel, choose Display/Undisplay Atoms from the Display menu (see Figure 5.10).

The Display/Undisplay Atoms panel is divided into two sections. Each section contains control for the following three operations.

- 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.

In the upper section, you can choose the atoms for the operation using picking tools, including a Pick option menu, an All button and the Atom Selection dialog box, which is opened using the Select button. You can also pick residues to display using the Display only this residue button in the toolbar:

In the lower section, you can apply the operation to the following structural units using the buttons under the operation heading:

- Protein Backbone
- Protein Sidechains
- Water Molecules
- Non-polar H Atoms
- Polar H Atoms

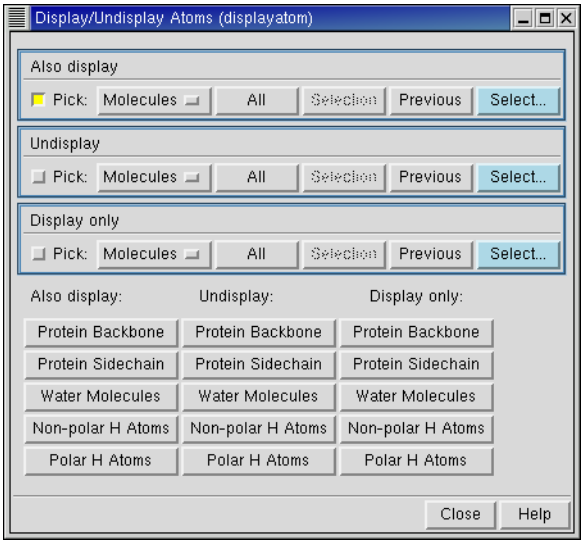


Figure 5.10. The Display/Undisplay Atoms ***panel.***

The tools in the lower section are also available from the toolbar as the Display Only, Also Display, and Undisplay button menus:

From these menus you can choose any of the structural units listed above, and you can choose All, All Hydrogens, or Select to open the Atom Selection dialog box and select the atoms to display or undisplay.

Manipulating Structures

Maestro provides a range of tools for manipulating structures in the Workspace. In addition to coordinate transformations such as rotation and translation, there are tools for centering a structure on a particular atom, zooming in on a structure, and arranging structures in a rectangular grid, which is called *tiling*.

Transformations can be carried out globally or locally. Global transformations move all of the atoms in the Workspace together as a unit. They do not change atom coordinates, only the orientation and location relative to the viewer. Local transformations move a user-defined subset of atoms relative to the rest of the atoms in the Workspace, and therefore must change the atom coordinates. Tiling also changes the atom coordinates.

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.

When a project is closed, the current rotation, translation, and zoom settings are saved with the project and restored when the project is opened.

6.1 Global Transformations

Global transformations are defined as rotation and translation of the entire structure or set of structures in the Workspace. The axes for rotation and translation are assigned to combinations of mouse buttons with the SHIFT and CTRL keys. These assignments are given in Table 6.1.

Global transformations do not actually change the coordinates of the structures in the Workspace. Rather, they change the view of the structures. You can save and restore a particular view of the structures from the toolbar—see Section 1.7.2 on page 15 for details. However, if you want to change the coordinates of the structures to reflect the new view, you can do so by choosing Update Coordinates from the Build menu.

To perform a global transformation, position the cursor in the Workspace, and hold down the relevant key and mouse buttons while you move the mouse. 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.

To select a new center that defines the axes for rotation, you can *spot-center* the molecule on an atom by right-clicking on the atom.

Table 6.1. Mapping of Workspace operations to mouse actions

Operation	Action
Rotate about the *x*- and *y*-axes	Drag with middle mouse button
Rotate about the *x*-axis only	Drag vertically with SHIFT and middle mouse button
Rotate about the *y*-axis only	Drag horizontally with SHIFT and middle mouse button
Rotate about the *z*-axis	Drag horizontally with CTRL 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 SHIFT and right mouse button
Translate along the *x*-axis	Drag horizontally with SHIFT and right mouse button
Translate about the *z*-axis	Drag horizontally with CTRL and right mouse button
Zoom	Drag horizontally with middle and right mouse buttons or with SHIFT+CTRL and middle mouse button

The other operation that does not change the coordinates of the structure is zooming, which is also performed with the mouse (see Table 6.1). You can also fit the displayed size of the structure to the Workspace by clicking the Fit to screen button on the toolbar.

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 workspace button in the toolbar

6.2 Local Transformations

A local transformation in Maestro is the movement of a user-defined atom subset[1] with respect to the other atoms in the Workspace, such as the movement of one molecule with respect to another. If you want to perform a translation, you need only select the atoms for transformation. If you want to perform a rotation, a rotation center is required. Maestro provides a default, but if this is not satisfactory, you must choose a rotation center.

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.

The controls for local transformations are available from the Advanced Transformations panel, which you open by choosing Global/Local from the Local transformation button menu in the toolbar.

The picking tools for defining atom sets are also available directly from this button menu. The selections you make in the Advanced Transformations panel persist, even when you alter the structures in the Workspace. To clear them, click Clear.

Local transformations are performed with the same combination of keys and mouse movements as global transformations. 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.

You can switch between global and local transformations by selecting Global or Local in the Rotation/Translation Scope section of the Advanced Transformations panel, by using the shortcut keys CTRL+G and CTRL+L in the Workspace, or by clicking on the Global/Local button on the toolbar. When the button is indented, local transformation is in effect.

While you are in local transformation mode, you can switch to global transformation mode temporarily by holding down the spacebar while you perform a transformation.

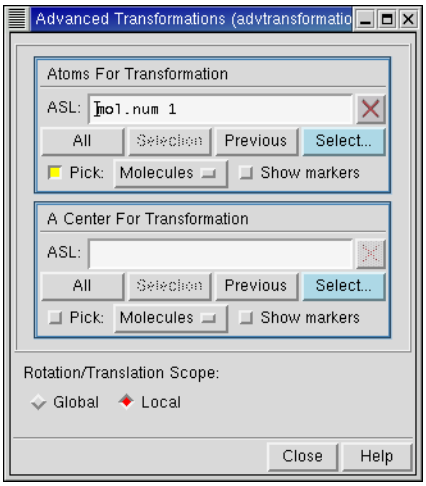


Figure 6.1. The Advanced Transformations ***panel.***

6.2.1 Selecting Atoms for Transformation

To select the atoms that you want to move, use the tools in the Atoms For Transformation section. You can pick atoms in the Workspace, click Select to select atoms using the Atom Selection dialog box, or enter an ASL expression in the ASL text box. You can also use the Local Transformation button menu to select an object and pick it in the Workspace.

If Show Markers is selected, the atoms are marked with yellow circles connected by yellow lines. Once you have started to select the atoms in the Atoms For Transformation section, the Local option in the Rotation/Translation Scope section is selected.

In order to see the atoms you want to pick for a local transformation, it may be necessary to rotate the structure. If this is the case, select Global in the Rotation/Translation Scope section, rotate the structure, then reselect Local to define atoms for local transformation.

If you want to translate atoms, you need not define a center for transformation. Once you have selected the atoms for transformation, you can perform the desired translation.

6.2.2 Selecting a Rotation Center

To perform local rotations, a center for rotation must be defined. By default, Maestro selects the centroid of the atoms selected for transformation as the rotation center. If Show Markers is selected, the rotation center is displayed in the Workspace as a purple ball. If the assigned centroid is not satisfactory, select a new center using the tools in the A Center For Transformation section. Displaying atom number labels may be helpful for determining which atom you would like to specify as the rotation center.

6.3 Tiling Multiple Entries

To arrange multiple included entries into a grid pattern in the Workspace, click the Tile Entries button in the toolbar.

This operation changes the coordinates of the structures in the entries. The entries are arranged according to the order they appear in the Project Table. To reverse this operation, choose Undo *action* from the Edit menu or click the Undo/Redo button in the toolbar.

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 Open/Close Project Table button in the toolbar.

The project data is stored in a directory whose basename 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 the directory specified by the environment variable `TEMP_PROJECT`. The default location is `$HOME/.schrodinger/tmp`.

This chapter discusses in some detail how to use the Maestro Project Facility.

7.1 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.

7.1.1 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 New from the Project menu. 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 an existing project, choose Open from the Project menu, or click the Open a project toolbar button.

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 7.1.4 on page 83.You can only have one project open at any time.

7.1.2 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 toolbar button.

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 7.1.4 on page 83. 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.

7.1.3 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 Unix shell 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.

7.1.4 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 operate like file selectors, but project selector filters are configured so that Maestro project directories (those with `.prj` extensions) are the only visible items. Most of the features of these panels are common to all operations. The panel features are described below.

Project Availability Indicators: Only one instance of a given project can be open at a time. To indicate whether a project is in use, an asterisk (`*`) is placed in front of each available project and an exclamation point (`!`) in front of each locked project. A project is locked if you or someone else already has the project open.

Directory selection buttons: In addition to the usual directory and file lists, there are two buttons for selecting directories: Launch Directory and Working Directory. The first selects the directory from which Maestro was launched, and the second selects Maestro's current working directory.

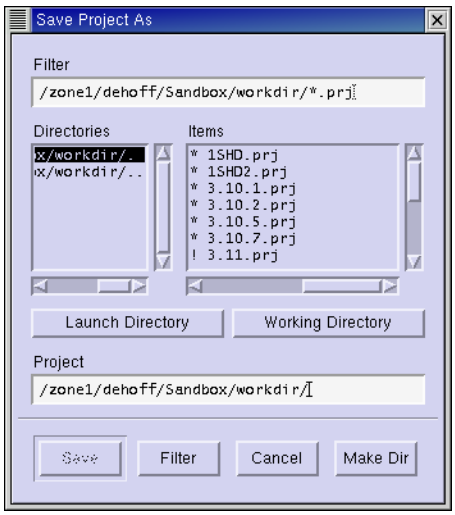


Figure 7.1. The Save Project as ***project selector.***

Options: When you merge projects you can choose to include any user-created files by selecting Include User Created Files.

Project Text Box: The Project text box is automatically populated with the name of the current directory. When you navigate to locate a directory, the text box is updated to reflect the current selection. If you are creating a new project, saving a scratch project or copying a project, enter the project name at the end of the text. You do not need to add the `.prj` extension, which Maestro supplies if it is absent.

Making New Directories: Some of the project selectors have been equipped with the ability to make new directories. The Make Dir button in these project selectors opens the Make Directory directory selector. To create a directory, navigate to the desired location and type the new directory name at the end of the path information in the Project text box. You can only create one new directory level at a time. To create multiple directory levels you must use this procedure for each level you want to create.

7.1.5 Annotating a Project

Because projects are frequently modified, it may be helpful to annotate your project. Maestro provides a project annotation feature that allows you to record notes about the project. To record notes, choose Annotation from the Project menu. The Project Annotation panel is displayed. You can enter new text or modify existing text in the text box. The date and time of project creation and each annotation is recorded by default, but this information can be modified or deleted.

7.2 Adding Entries to a Project

Projects are made up of entries. Entries can contain multiple structures and their properties. Each entry has both a name, by which it is identified internally and which can be modified by Maestro, and a title, which can be set or changed by the user but is otherwise not modified by Maestro.

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 Table.

7.2.1 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, MacroModel, 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 Chapter 2 for more information on importing structures.

7.2.2 Creating Entries From Workspace Structures

When you build structures in the Workspace from scratch, these structures constitute a scratch entry, and are not saved in the project. To save the scratch entry in the current project, choose Create Entry From Workspace from the Project menu, and type an entry name in the dialog box that is displayed. If you choose an existing entry name, Maestro appends `-wse`*n* to the entry name to ensure that the name is unique, where *n* is a number starting from 1. All structures in the Workspace are placed in the entry that you create. You can also create an entry using the Create entry from Workspace button in the toolbar.

7.2.3 Incorporating Entries From Job Output

When you use selected or included entries from a project as input for a MacroModel, Basic Impact, QSite, or QikProp job, 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. When you use entries for a Jaguar job, the results are automatically incorporated by appending new entries. Incorporated entries have `-inc`*n* appended to the entry name, where *n* is a number starting from 1.

For more information on incorporating job output into the Project Table, see section Section 14.7 on page 191.

7.2.4 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.

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.

If none of the incoming entries has a name identical to an entry in the current project, the entry names remain intact. If there are duplicate entry names in the projects to be merged, the Entry Name Resolution panel is displayed, and you must choose a resolution scheme in the Retain Entry Names In section—Current, Incoming, or User Specified. If you select Current, the names in the current project are kept, and the conflicting incoming entries are renamed. Likewise, if you select Incoming, the incoming entries retain their names, and the conflicting entries in the current project are renamed. If you want to choose which entries to rename, select User Specified, then click the Specify button. The User Specified Conflict Resolution panel is displayed, and you can choose to rename either the current or the incoming entry.

The resolution scheme that Maestro offers may not produce especially meaningful names. For example, if in both the current and the merge source project, you have entries named `entry`, and you already have other entries in the current project named `entry-1`, `entry-2`, and `entry-3`, Maestro renames the incoming `entry` as `entry-4`. Since renaming entries in this fashion may destroy any location cues that you were using, you may want to go into each project separately and resolve any naming conflicts before attempting to merge projects. However, the titles of the entries are preserved, and these can be used to distinguish entries when the entry name is changed by Maestro.

7.3 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, a toolbar, and the Project Table itself. 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. Each row contains the row number, an icon in the In column indicating whether the entry is displayed in the Workspace, the title, a button to open the Surfaces panel if there are surfaces associated with the entry, the entry name, and any properties associated with the entry. The first four columns of the project table are always visible: the row number, the In column, the entry name or the title (you can exchange these two from the Table menu), and the Surf column. The remainder of the columns appear in the scrolling section of the table.

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 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 inclusion state is indicated in the In column. Excluded entries—entries that are not displayed in the Workspace—are marked with an empty diamond. Included entries are

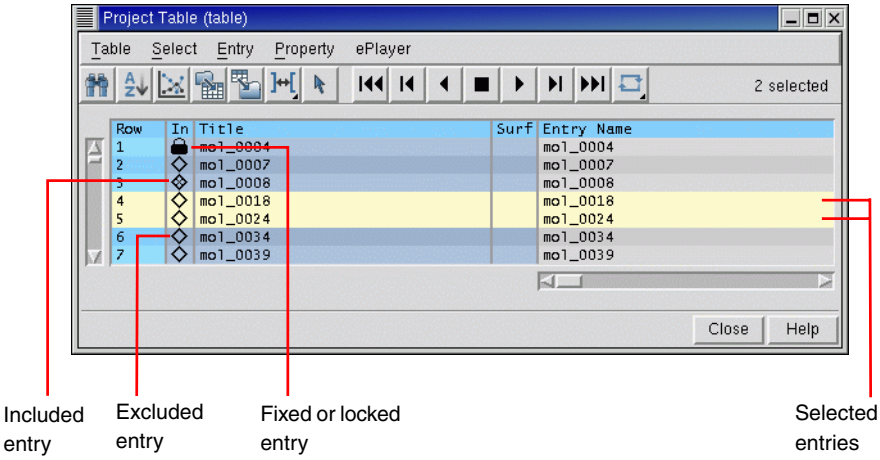


Figure 7.2. The Project Table ***panel.***

marked with a cross in the diamond. 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 selection and inclusion states are stored in the project, so they are persistent.

7.3.1 The Project Table Toolbar

The toolbar contains two groups of buttons and a status display. The first set of buttons opens various panels that allow you to perform functions on the entries in the project table. The second set of buttons controls the ePlayer, which "plays through" the selected structures: each structure is displayed in the Workspace in sequence, at a given time interval. A description of the toolbar buttons is provided below. The use of these buttons is also discussed in later sections of this chapter.

Find
Open the Find panel for locating alphanumeric text in any column of the Project Table, except for the row number.

Sort
Open the Sort Project Table panel for sorting entries by up to three properties.

Plot
Open the Plot XY panel for plotting entry properties.

Import structures
Open the Import panel for importing structures into the project.

Export structures
Open the Export panel for exporting structures to a file.

Columns menu
Choose an option for adjusting the column widths.

Entry selection
Open the Entry Selection dialog box for selecting entries based on criteria for entry properties.

Go to start
Display the first selected structure.

Previous
Display the previous structure in the list of selected structures.

Play backward
Display the selected structures in sequence, moving toward the first.

Stop
Stop the ePlayer.

Play forward
Display the selected structures in sequence, moving toward the last.

Next
Display the next structure in the list of selected structures.

Go to end
Display the last selected structure.

ePlayer loop menu
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.

7.3.2 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 configure the Project Table.
- Select—select all entries, none, invert your selection, or select classes of entries using the Entry Selection dialog box and the Filter panel.
- Entry—include or exclude entries from the Workspace, display or hide entries in the Project Table, and perform various operations on the selected entries.
- Property—display and manipulate entry properties in the Project Table.
- ePlayer—view entries in succession, stop, reverse and set the ePlayer options.

7.3.3 Mouse Functions in the Project Table

The standard use of shift-click and control-click to select objects is supported in the Project Table. This behavior applies to selection of entries and inclusion of entries in the Workspace. Dragging to resize rows and 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 7.5.8 on page 97 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.

A summary of project-based mouse functions is provided in Table 7.1.

Table 7.1. 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.
Include an entry, exclude all others.	Click the In column of the entry.
Move selected entries.	Drag the entries.

Table 7.1. Mouse operations in the Project Table (Continued)

Task	Mouse Operation
Paste text into a table cell.	Middle-click.
Resize rows or columns.	Drag the boundary with the middle mouse button.
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 the entry or the In column.

7.3.4 Project Table Shortcut Keys

Some frequently used operations have been assigned shortcut key combinations. The shortcuts, their functions, and their menu equivalents are listed in Table 7.2.

Table 7.2. Shortcut keys in the project facility

Keys	Action	Menu Equivalent
CTRL+A	Select all entries	Select > All
CTRL+F	Fix entry in Workspace	Entry > Fix
CTRL+I	Show import panel	Table > Import Structures
CTRL+N	Include only selected entries	Entry > Include Only
CTRL+U	Deselect all entries	Select > None
CTRL+X	Exclude selected entries	Entry > Exclude
CTRL+Z	Undo/Redo last command	Edit > Undo/Redo in main window

7.3.5 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.

Displaying a subset of entries. You can display a subset of entries by selecting the entries, then choosing Show Only from the Entry menu, and likewise you can hide the selected entries by choosing Hide from the Entry menu. To redisplay all entries, choose Show All from the Entry menu.

Displaying a subset of properties. You can display a subset of properties by choosing Show from the Property menu, 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.

Resizing rows and columns. You can resize rows or columns by dragging the border of the row or column using the middle mouse button. You can also set the width of the columns to the width of the widest data item, the width the widest of the data and the heading, or to a fixed width, by choosing from the Columns button menu on the toolbar or the Columns submenu of the Table menu.

Swapping Title and Entry name. In the non-scrolling area of the project table, you can display either the title or the entry name. You can swap these two from the Columns submenu of the Table menu.

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.

7.3.6 Finding Text in the Project Table

If you want to locate text in the Project Table, whether it is a string or a numerical value, choose Find from the Table menu. The Find panel is displayed. Enter the text you want to find, select Down to search down from the first entry or Up to search up from the last entry, and click Find Next. The Project Table scrolls to the found entry, but the entry is not selected.

To increment the search, click Find Next again. The Project Table scrolls to the next instance of the search string. If it finds none, the Project Table beeps as reaches the end (or beginning) of the table and scrolls to the original found entry.

Note: If you click on the Project Table panel, then click Find Next, the search starts over, searching from the beginning of the table if Down is selected, or from the end of the table if Up is selected.

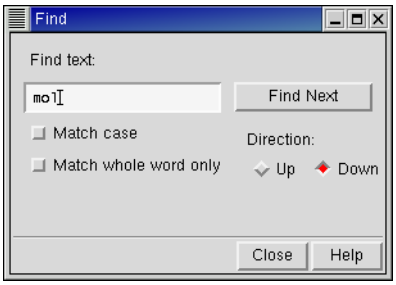


Figure 7.3. The* Find *panel.

7.4 Selecting Project Entries

Selection is the action of 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 86. 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 7.1, Maestro provides additional capabilities for selecting entries based on their properties.

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 7.2 on page 90.

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.

7.4.1 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. 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*.

7.4.2 The Entry Selection Dialog Box

The Entry Selection dialog box (Figure 7.4) 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 or using the Select Only toolbar button.

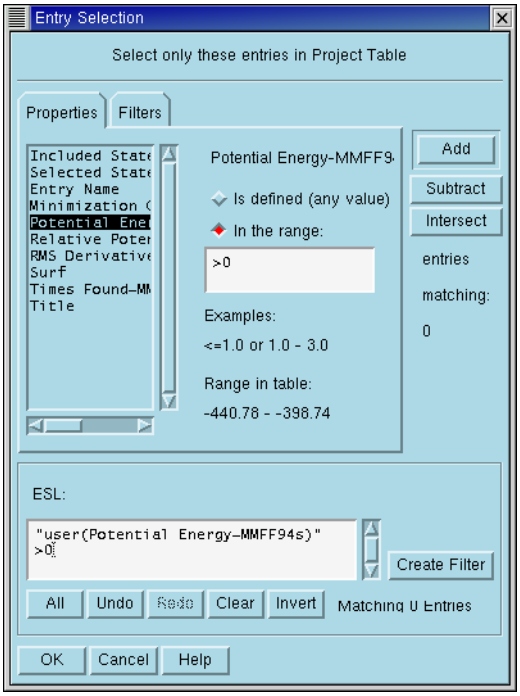


Figure 7.4. The Entry Selection ***dialog box.***

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 folders, 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 folder, then select a condition from the right side of the folder. 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 numerical (real or integer) properties, the value lies in a given range, for example, >= 5.0 or 1 - 7. You can use any of the six operators ==, !=, <, >, <=, and >= to define the range of property values.
- For textual 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.
- For Boolean properties, the value is true or false.

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.

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 folder of the Entry Selection dialog box and on the Filter submenu of the Select menu.

7.4.3 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 9.2.4 on page 123 for more information.

7.4.4 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, and * is a wildcard character that represents any string.
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.

7.5 Operating on Selected Entries

The Entry menu provides tools to perform various operations on the selected table entries. These operations are discussed in the following sections.

7.5.1 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 9.2.5 on page 123 for more information.

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 press CTRL+F. These entries remain in the Workspace until you explicitly exclude them.

7.5.2 Limiting the Number of Entries Displayed

In large projects you may want to limit the number of entries displayed in the Project Table. To do this, select the entries, then choose Show Only from the Entry menu. Likewise you can hide the selected entries by choosing Hide from the Entry menu. To redisplay all entries, choose Show All from the Entry menu. The display of entries does not affect either the subsequent selection or inclusion of entries—though of course you can only use the mouse to select or include the entries that are displayed in the Project Table.

7.5.3 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 base 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.

   Maestro automatically adds incremental numbers to the name you assign, to make the entry names unique.

7.5.4 Duplicating Entries

To duplicate entries, select the entries and choose Duplicate from the Entry menu. Maestro copies the entries to the end of the Project Table. The new entries retain the same base name as the originals, but have `-dup`*n* appended. The number *n* indexes the duplicates. The title is preserved when the copy is made.

7.5.5 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 Merge from the Entry menu. The first new entry in a session is automatically named `merge`. Subsequent combination entries are named `merge.mrg1`, `merge.mrg2`, etc. When you merge entries, Maestro places the new entry after the last entry that was included in the merge operation. The new entry inherits the title from the first selected entry.

7.5.6 Splitting Entries by Molecule

Entries that contain multiple molecules can be split into entries that contain individual molecules. For example, you can split a protein-ligand complex into separate entries for the protein and the ligand. To split an entry, select it and choose Split by Molecule from the Entry menu. When an entry is split, a copy of the original entry is kept, and a new entry is created for each molecule in the original entry. The exception is that water molecules are collected in a single entry, with the suffix `-waters` appended to the original entry name. The new entries retain the same base name as the original entry, with `-dis`*n* appended. The number *n* indexes the new entries.

7.5.7 Deleting Entries

You can delete entries from the Project Table by selecting the entries, then choosing Delete from the Entry menu or pressing DELETE. The entries disappear immediately: you are not prompted to confirm your choice. However, this function is undoable by selecting Undo entry-delete from the Edit menu of the Maestro main window.

7.5.8 Moving Entries

Entries in the Project Table can be moved to another location in the list. 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.

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, or choose to move the rows to the beginning or the end of the table.

7.5.9 Sorting the Entries of a Project

You can sort all entries or the selected 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.

To sort entries by a single property, right-click and hold in the property header and choose Sort from the menu that is displayed.

To sort entries by more than one property, you can use the Sort Project Table panel. In this panel you can choose from three sort keys to sort the entries, and for each key you can choose to sort in ascending or descending order.

To sort entries:

1. Select the desired entries.
2. Choose Sort Selected Entries from the Table menu or click the Sort toolbar button.

   The Sort Project Table panel is displayed.
3. Select a property from the Primary Key list.
4. If you want to sort entries whose primary key is the same by another property, select a property from the Secondary Key list, and likewise for the Tertiary Key list.
5. Select Ascending or Descending for each key for which you made a selection.
6. Click Sort Selected Rows or Sort All Rows.

If three keys is not sufficient to sort the table in the way you want, you can use the `tablesortfields` command in the Command Input Area to choose as many keys as you want. See the *Maestro Command Reference Manual* for the command syntax.

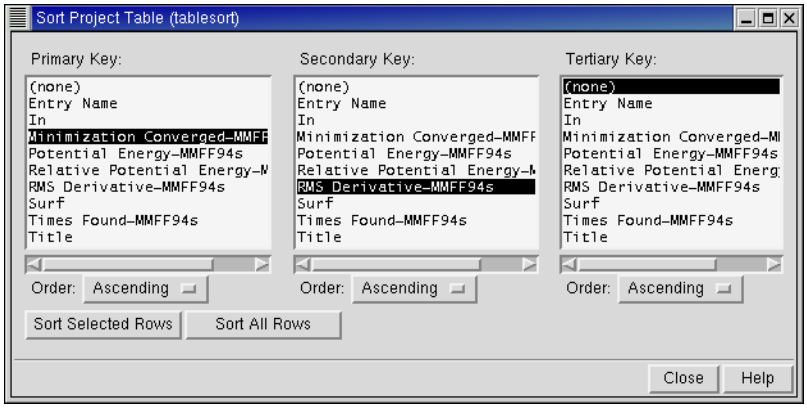


Figure 7.5. The Sort Project Table ***panel.***

7.6 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. 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.

7.6.1 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, or the Next and Previous items on the ePlayer menu.

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. 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 redisplays 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.

7.6.2 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.

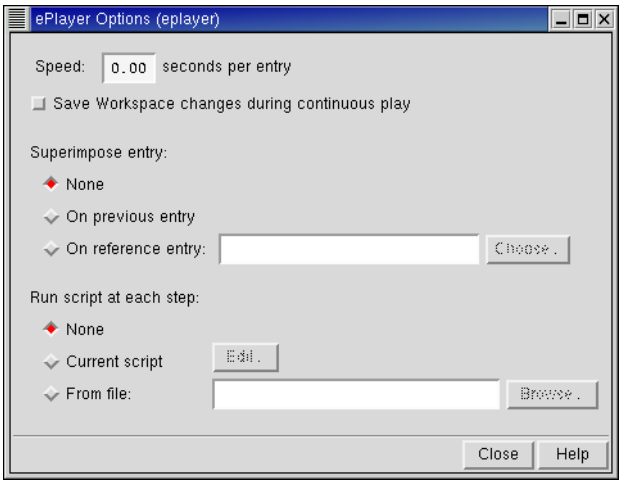


Figure 7.6. The** ePlayer Options **panel.

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.

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.

7.7 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 2.3 on page 27 and Section 2.4 on page 28 for information on exporting and importing properties.

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.

7.7.1 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 property values. A third is to calculate one of a selection of new properties.

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 7.7). 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.

To create a new property by copying an existing property, choose Copy from the Properties menu 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 the next section for more information on copying properties.

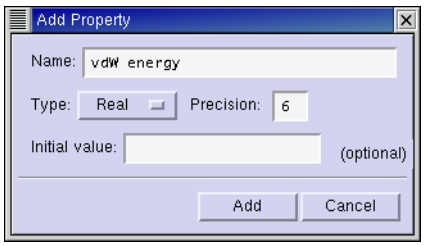


Figure 7.7. The** Add Property **panel.

Maestro provides a selection of properties that can be calculated for the entry from the structure itself. These calculations are done from the Calculate Properties panel, which you open by selecting Calculate from the Property menu. The available properties, given in the Properties list at the top of the panel, are:

- Number of atoms
- Number of residues
- Number of molecules
- Molecular weight
- Molecular formula
- Molecular charge
- Secondary structure content
- Substructure

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. Information on Maestro substructure notation is contained in the file `$SCHRODINGER/services-v`*version*`/doc/mmsubs_syntax.txt`.

For some properties, there are options or settings that must be made in order to calculate the property. These are available in the area below the property list. To calculate the property, select it in the Property list, select any options and enter any data in the section below the list, select a Calculate For Entries option (All or Selected), then click Calculate.

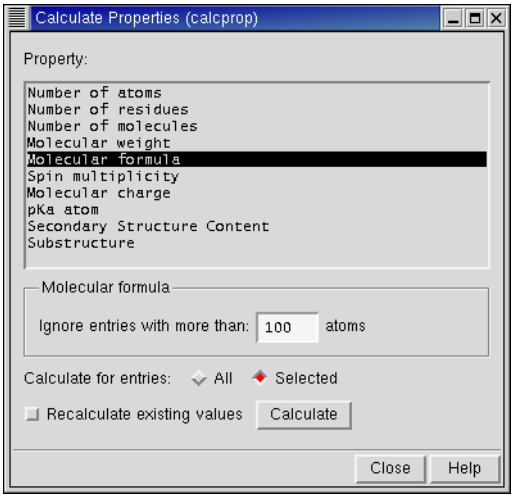


Figure 7.8. The Calculate Properties ***panel.***

If you have previously calculated the property for some entries and want to calculate it for other entries, you can choose to recalculate the existing values by selecting Recalculate existing values.

7.7.2 Changing Property Values

Maestro provides several means of changing the values of properties. You can edit individual cells and the selected cells of a single column, and you can copy values from another property.

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.

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 Entry Name, In, Surf, and Selected. These property values cannot be deleted. The Surf property cannot be overwritten. The Entry Name can only be replaced by a legal entry name. If the name is legal but not unique, it is made unique and a prompt to accept the modified name is

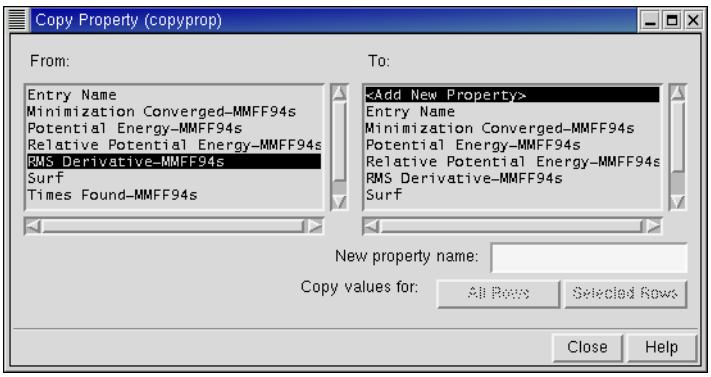


Figure 7.9. The Copy Property ***panel.***

displayed. If the source value is missing or the conversion fails when copying to the In or Selected properties, these properties are set to false. In addition, the Title property is required by Maestro, so if you delete it, Maestro creates a replacement title property.

The following conditions determine what happens when the destination is not one of the four 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.

7.7.3 Renaming and Deleting Properties

You can rename and delete properties other than the fixed properties, Entry Name, In, Surf, Title, and Selected. To rename a property, you can edit the table cell directly by clicking in the cell, changing the text, and pressing ENTER or clicking elsewhere in the Project Table. You can also rename properties by choosing Rename from the Property menu, and editing the name in the Rename Property panel.

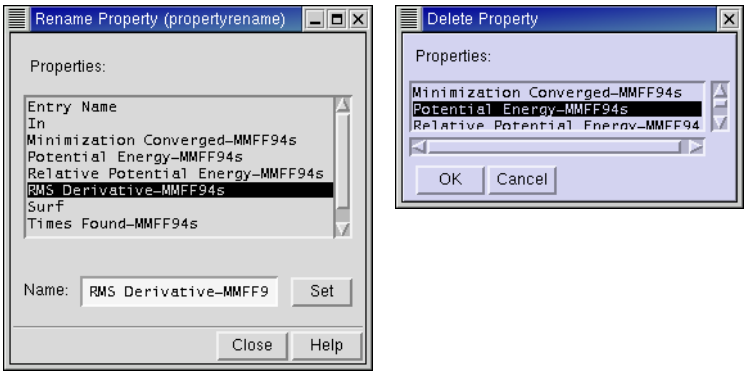


Figure 7.10. The Rename Property ***panel and the*** Delete Property ***dialog box.***

To delete a property, choose Delete from the Property menu to open the Delete Property dialog box, select the properties in the list and click OK. You can choose multiple properties by shift-clicking and control-clicking the properties.

7.7.4 Displaying Selected Properties

If you want to limit the number of properties displayed, you can select the properties to be displayed in the Show Property dialog box. To open this dialog box, choose Show from the Property menu. You can select multiple properties in the Properties to show list by shift-clicking and control-clicking the list items.

Below this list is a set of tools for selecting properties. Select All selects all properties in the list and Clear clears the list. In the Property Family section, you can select properties that were generated by one of the computational programs, such as QikProp, or user-generated properties—properties that you added. Click Add to add properties of that family to the selection. Click Remove to remove properties of that family from the selection.

When you have chosen the properties, click Show to change the Project Table display. You can redisplay all properties by choosing Show All from the Property menu on the Project Table.

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 spreadsheet file.

7.7.5 Moving and Resizing Property Columns

You can move and resize individual columns in the project table with the mouse. Dragging a column border with the middle mouse button resizes the column. Dragging the column heading moves the column. You can only move columns that are in the scrollable area. By default, the Title property is in the fixed area and the Entry Name property is in the scrollable

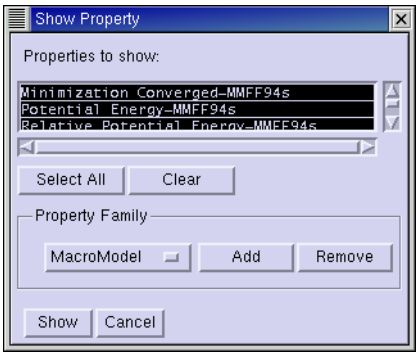


Figure 7.11. The Show Property ***dialog box.***

area. You can swap these two columns by choosing Swap Title/Entry from the Columns submenu of the Table menu.

You can also 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.

7.7.6 Exporting and Importing Data

Maestro does not provide 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 2.3 on page 27 and Section 2.4 on page 28.

To specify a filename for the exported data, type a name in the File text box. To export the file to Maestro's current working directory, click Export. To export to a different directory, click Export To and navigate to another directory.

7.8 Undoing Project Operations

All changes made directly to the Project Table are saved immediately, regardless of your synchronization preference setting. The synchronization setting affects only the changes made in the Workspace. (For more information about synchronization preferences, see Section 11.2.2 on page 144.) You can save a copy of your project using Maestro's Snapshot feature before performing operations that you might want to undo. To generate a snapshot of the current project, choose Make Snapshot from the Project menu.

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 may be prompted to do so. Otherwise, the Make Snapshot command is executed immediately and you receive no notification other than the temporary display of the cursor as a stopwatch.

Only one snapshot can be preserved at a time. Any previous snapshots are overwritten when you issue the Make Snapshot command.

To revert to the snapshot you made, choose Revert to Snapshot from the Project menu.

If you want to discard all work done to a particular project during a Maestro session, you can revert to the opening state of a project, which is saved by Maestro. Like reverting to a snapshot, reverting to the opening state of a project discards all work performed on that project since it was last opened in the current Maestro session. To scrap the project in its present state and begin again, choose Revert to Opening State from the Project menu. Since the reversion is not undoable, you will be prompted to confirm your choice.

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 9) are discussed elsewhere, most of the tools are discussed here.

8.1 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. 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 undisplay their associated markers when you close the panel. The exception is measurement markers, which are displayed even if the Measurements panel is hidden.

To display the markers for a particular operation, select Show Markers in the panel used to perform the operation.

8.2 Making Measurements in the Workspace

The Measurements panel (see Figure 8.1 on page 110) provides tools to determine the geometric relationships between atoms in the Workspace. These tools are contained in five folders—Distances, Angles, Dihedrals, H-Bonds, and Contacts.

To open the Measurements panel, choose Measurements from the Tools menu.

8.2.1 Measuring Distances, Angles, and Dihedrals

The controls for Distances, Angles, and Dihedrals 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.

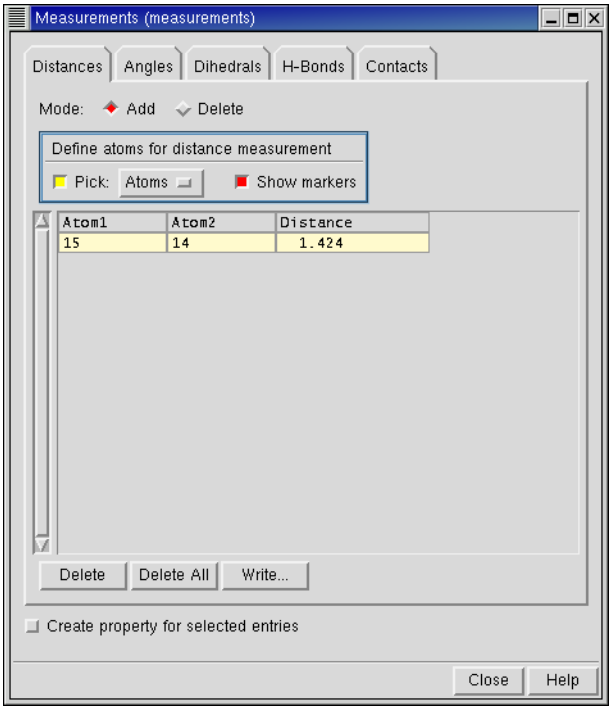


Figure 8.1. The Distances ***folder of the*** Measurements ***panel.***

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 Show 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.

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 Show 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. You can also select the Delete option under Mode and click the defined atoms in the Workspace to delete a measurement.

You can also make measurements using the Measure distances, angles or dihedrals toolbar button.

To make a measurement, choose Distance, Angle, or Dihedral 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.

8.2.2 Displaying Hydrogen Bonds and Contacts

The procedures for displaying H-Bonds and Contacts are similar. Unlike distance, angle, and dihedral measurements, you can display hydrogen bonds and contacts for an unlimited number of atoms, and you define the desired atoms by placing them in sets. Two sets can be defined at any given time, and you can choose to display the hydrogen bonds or contacts between the atoms of a set or between the two separate sets.

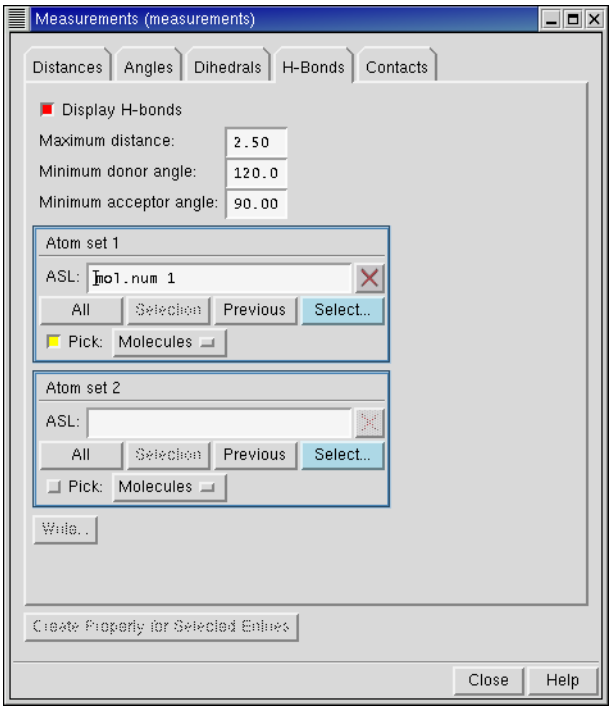


Figure 8.2. The H-Bonds ***folder of the*** Measurements ***panel.***

To see hydrogen bonds or contacts marked in the Workspace, select Display H-bonds or Display Contacts. For contacts, you must also select the type of contact—Good, Bad, or Ugly—that you want to measure.

Default criteria for defining hydrogen bonds or contacts are given in the text boxes at the top of the folder. To change these criteria, enter a new value in the relevant text box. For hydrogen bonds you can set the Maximum distance, Minimum donor angle and Minimum acceptor angle. For contacts, you can alter the contact cutoff ratios in the Good contacts, Bad contacts, or Ugly contacts text boxes.

To define an atom set, use the picking tools, click Select to open the Atom Selection dialog box, or enter an ASL expression in the ASL text box. If you define only Atom set 1, the H-bonds or contacts are displayed within that set. If you define both Atom set 1 and Atom set 2, the H-bonds or contacts are displayed between the two sets.

When you have finished measuring, click Clear in each of the atom definition sections.

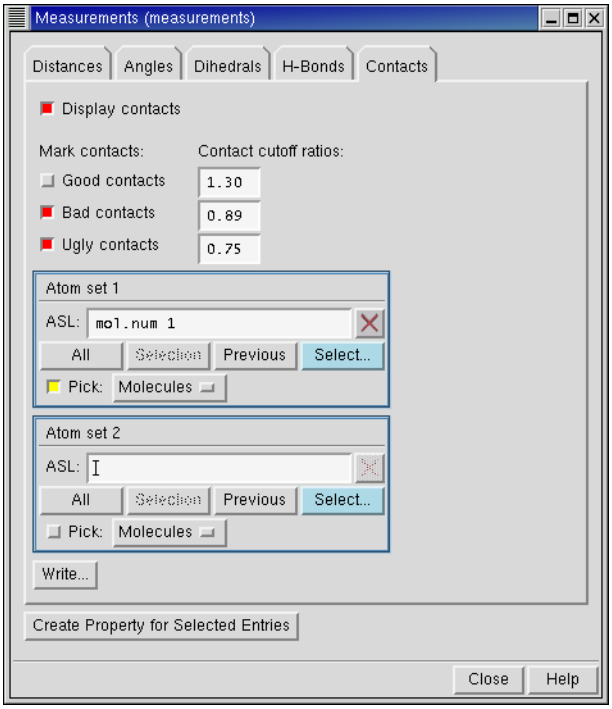


Figure 8.3. The Contacts ***folder of the*** Measurements ***panel.***

You can also display hydrogen bonds from the toolbar. First, choose Inter H-bonds or Intra H-bonds from the Display H-bonds button menu:

Then select a molecule in the Workspace. If you choose Inter H-bonds, hydrogen bonds between the selected molecule and the rest of the atoms in the Workspace are displayed. If you choose Intra H-bonds, hydrogen bonds within the selected molecule are displayed.

8.2.3 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 measured 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. For hydrogen bonds and contacts, the property is the number of H-bonds or contacts.

Each folder 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, the numbering of the atoms, 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.

8.2.4 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 Draw mode in the Build panel 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 folder of the Build panel. If you attach the dummy atom to your structure, you can adjust its position using the Adjust panel.

8.3 Superimposing 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 display the structures in the Workspace and then use the tools in the Superposition panel to evaluate the differences in the atom positions. Each structure must be in a separate project entry.

The superposition scheme works by aligning the first selected atom in each structure, then attempting to align the second selected atom, and so on. 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.

To open the Superposition panel, choose Superposition from the Tools menu.

To superimpose all the displayed structures, click All in the Superimpose by ASL section. 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 same way, which usually requires that the entries be conformers. 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.

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.

If you want to compare more than two structures or if picking individual pairs is not practical, you can superimpose atoms defined by an ASL expression. To do so, click Select and construct the expression using the tools in the Atom Selection dialog box, or enter the expression in the Superimpose by ASL text box. For example, to apply the superposition operation to only carbon atoms, type `atom.e C` and press ENTER. For more information on the Atom Selection Language, see the *Maestro Command Reference Manual*.

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.

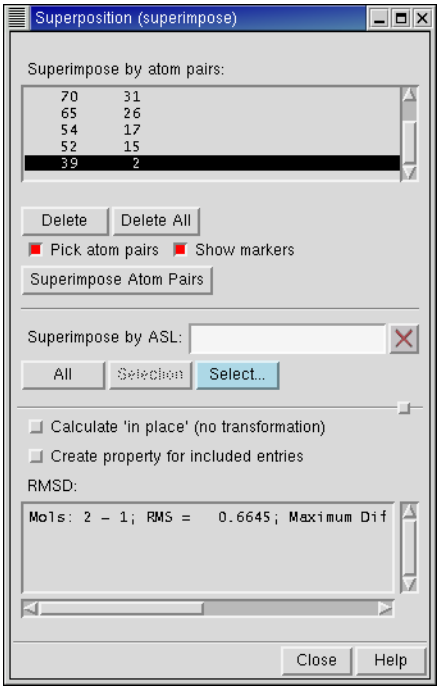


Figure 8.4. The Superposition ***panel.***

If you do not use the calculate in place option, you can separate the superimposed entries by clicking the Tile Entries button in the toolbar.

The entries are aligned in a grid, but they are not returned to their original coordinates. If you do want to return the structures to their original positions, you must define an Undo block before starting the superposition. For more information on Undo blocks, see Section 1.7.1 on page 15.

You can store the RMS deviation as a property for each entry that was superimposed. To create a property, select Create property for included entries before you perform the superposition. The property is labeled RMSD *entry-name* or RMSD In Place *entry-name*, depending on how you performed the superposition. The reference entry has a value of zero for this property. The reference entry name is used for *entry-name* 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 7.7.3 on page 105 for information on renaming properties.

8.4 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 Sets from the Tools menu.

8.4.1 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.

8.4.2 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 ASL text box, or click Select to select atoms using 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.

If you select Show 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.

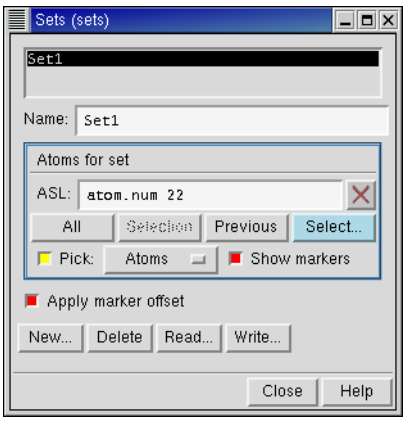


Figure 8.5. The* Sets *panel.

For more information on ASL, see the *Maestro Command Reference Manual*, Chapter 3. For more information on the Atom Selection dialog box, see Section 4.3 on page 57.

8.4.3 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.

The procedure to read an existing sets definition file is similar. 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.

8.5 Assigning and Aligning Protein Structures

Maestro has tools for aligning protein structures and for assigning secondary structures in 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, which you open from the Tools menu. To use this panel, you must have a Prime license. For information on this panel, see the *Prime User Manual* or the online help for the panel.

The Assign Secondary Structure command on the Tools menu provides a way of assigning secondary structure 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.

Plotting

Maestro's Plot Facility allows you to generate XY plots of any two columns of data in the Project Table. Multiple plots are supported, and plot data is stored inside the project. When you have created a plot, you can select data points in the plot and display the corresponding entries in the Workspace.

9.1 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. To create a new plot, first select the entries in the Project Table whose data you want to plot, then choose Plot from the Table menu or click the Plot button on the toolbar.

The Plot XY panel is displayed with a blank plot area. Now choose New Plot from the Plot menu. The New Plot dialog box is displayed.

To assign a name to the plot, enter a name in the Plot Name text field. The name appears in lists used to select plots, in the caption name underneath the plot, and in any TIFF or JPEG images that you make of the plot.

You can plot more than one set of data in a single plot. To distinguish the data sets, or *series*, enter a name in the Series Name text field. To create new series, however, you must use the New Series dialog box. See Section 9.3.2 on page 125 for more information.

When you have assigned names, choose the property to be plotted on each axis from the X Property and Y Property lists.

The default plot type is a line plot. If you want to generate a plot of frequency of occurrence of a range of values against the midpoint of the value range, select Frequency Plot. An extra section is displayed. In this section you can choose to display the frequency on the x-axis or the y-axis. You can only choose one property for a frequency plot. The property that you select is divided evenly into ranges based on the maximum and minimum values of the property and the number of buckets you enter in the Buckets text box.

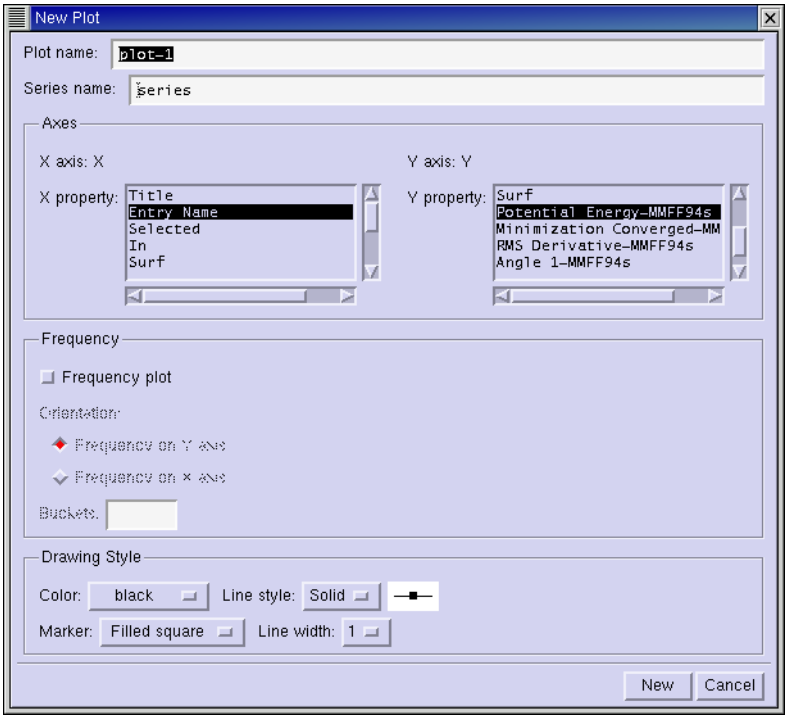


Figure 9.1. The New Plot ***dialog box.***

You can modify the appearance of the data point markers and the plot line using the option menus in the Style of Drawing section: Color, Marker, Line Style, and Line Width.

When you have finished characterizing the plot, click New. The Plot XY panel is updated with the new plot.

9.2 Viewing and Manipulating Plots

The Plot XY panel is used to add, edit, view, and delete XY plots. To open the Plot XY panel, choose Show Plots from the Selection menu of the Project Table panel.

Plots are displayed in the main window of this panel. Plots can be tiled, or can be arranged either horizontally or vertically in the window. You can display as many plots as you like in the Plot XY panel, but with the addition of each plot, all plots are reduced in size.

The zoom bar is the area at the right of the Plot XY panel. It contains controls for zooming and panning the selected plots. You can display it or hide it by selecting Plot Zoom Bar from the Settings menu.

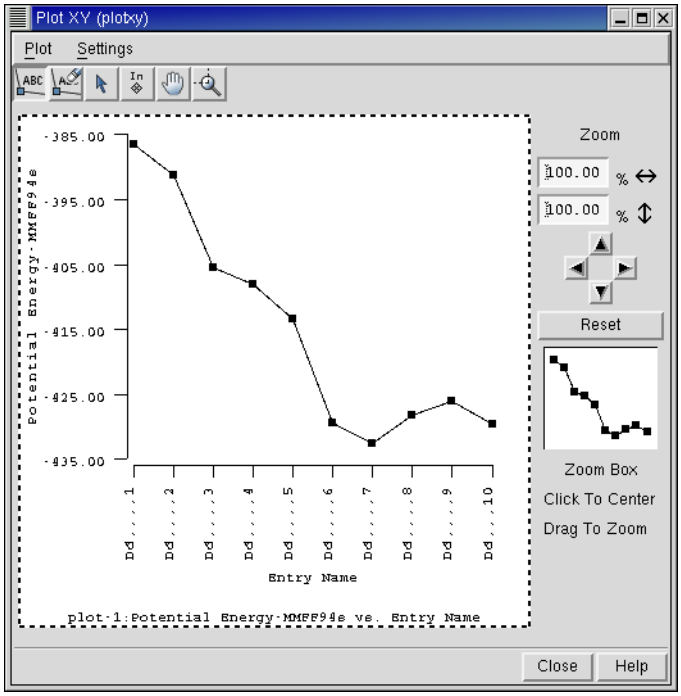


Figure 9.2. The Plot XY ***panel.***

The Plot toolbar contains buttons for operations on the selected plot, such as labeling and unlabeling data points, selecting and deselecting entries associated with data points, including and excluding entries associated with data points, panning the plot, and zooming in on the plot.

9.2.1 Selecting Plots

You can select a plot by clicking in it. The selected plot is outlined with a dotted line. You can select more than one plot by clicking in the first plot and shift-clicking in additional plots. Once you have multiple plots selected, you can control-click in a plot to remove it from the selection. To select all plots, press CTRL+A; to deselect all plots, press CTRL+U.

You can also select plots from the Plot menu or from the list of plots in the Plot Settings panel. To open this panel, choose Plot Settings from the Settings menu or press CTRL+P.

As with entries in the Project Table, you can select plots and display plots independently. When you have selected a group of plots, you can display only those plots, add them to the display, or remove them from the display by using the commands on the Plot menu.

9.2.2 Panning and Zooming

The zoom bar controls operate on one or more selected plots. If you do not have any plots selected, then none of the zoom bar controls are active. If you have one plot selected, then the zoom controls display the plot's current zoom. If you have more than one plot selected, and all of the plots have the same zoom, that zoom is displayed. Otherwise, the zoom controls are blank. When you have multiple plots selected, the panning and zoom controls operate within each plot to pan the plotted data with respect to the axes, or zoom in on the plotted data.

The first items in the zoom bar are edit controls for directly setting the zoom for both horizontal and vertical directions. Below the edit controls are a series of arrow buttons for panning the displayed region of the selected plots. Following the arrow buttons is a Reset button. This button restores the selected plots to their initial full-scale setting of 100% zoom and no panning. The final section of the zoom bar is the Zoom Box—a control for directly setting the zoom and pan relative to an image of the plot's data. This control is only active if you have a single plot selected. If you have no plots selected, or more than one plot selected, this control is blank. If the Zoom Box is active, you can use it to display only a portion of the selected plot. To change the current view of the plot, click inside the Zoom Box to center the view on that location. To zoom in, drag the mouse. The selected plot is zoomed to show only the rectangle defined by the mouse.

If you want to pan or zoom in on a single plot using the mouse, you can use the Pan plot and Zoom box buttons in the tool bar:

To pan a plot, click the Pan plot button, then drag the mouse in the plot in the desired direction. The data follows the mouse movement. To zoom in on a plot, click the Zoom box button, then drag the mouse over the region you want to zoom in on. When you release the mouse button, the plot zooms in to the defined region.

9.2.3 Labeling and Unlabeling Data Points

You can add labels to data points, or delete them, by clicking either the Label Points button or the Unlabel Points button, which are shown below.

To label points, click the Label Points button, then click a data point. The Label Points dialog box opens. In this dialog box you can label the point with any combination of: the corresponding entry name, the x-axis property value, and the y-axis property value. To remove data point labels, click Unlabel Points, then click on the labeled point.

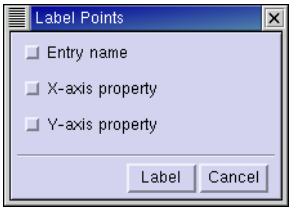


Figure 9.3. The Label Points ***dialog box.***

9.2.4 Selecting and Deselecting Project Entries

If you click the Select entry button, shown below, clicking on a data point in the selected plot selects or unselects the corresponding entry in the Project Table. The usual rules for selection apply to selecting data points: clicking on its own includes one entry and excludes all others, shift-clicking includes an entry with the other included entries, and control-clicking includes or excludes the entry. You can also select multiple data points and their corresponding entries by dragging. All the data points in the bounding box have their entries selected or unselected in the Project Table.

9.2.5 Including and Excluding Project Entries

If you click the Include entry button, shown below, clicking on a data point includes the corresponding entry in the Workspace. The usual rules for selection apply to selecting data points: clicking on its own includes one entry and excludes all others, shift-clicking includes an entry with the other included entries, and control-clicking includes or excludes the entry. You can also select multiple data points and their corresponding entries by dragging. All the data points in the bounding box have their entries included in the Workspace.

9.3 Editing Plots and Plot Settings

The Plot Settings panel is used to select plots, edit plot properties, edit X and Y axes, and add, edit, and delete data series. To open the Plot Settings panel, choose Plot Settings from the Settings menu of the Plot XY panel or press CTRL+P. You can select multiple plots in the list of plots, but you can only change the settings when you have a single plot selected.

9.3.1 Modifying Plot Attributes

The tools in the Plot folder allow you to modify plot attributes other than the plot line.

Displaying and Undisplaying a Plot: To display a plot, select Plot displayed. To hide a plot, deselect Plot displayed.

Modifying a Plot Caption: When you create a new plot, a caption is displayed underneath the plot in the Plot XY panel by default. The default caption contains the assigned caption text as well as the plot name. To modify the caption content, type the new caption in the Caption text box. To change the contents or placement of the caption, or to undisplay the caption, select the appropriate options.

Displaying Selection and Inclusion Markers: By default, points corresponding to selected and included entries are not marked. To display the markers, select Display selected entry markers or Display included entry markers.

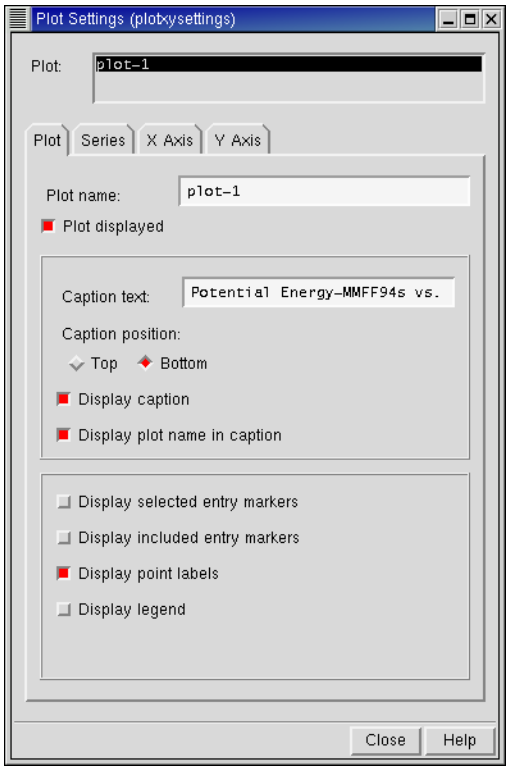


Figure 9.4. The Plot ***folder of the*** Plot Settings ***panel.***

Displaying Data Point Labels: If Display point labels is selected, labels are displayed for data points that have labels. For frequency plots, currently, only the exact position of the point on the x-axis is available.

Displaying a Plot Legend: To display a plot legend that shows which lines and points correspond to each data series, select Display legend.

9.3.2 Operating on Plot Series

The tools in the Series folder allow you to manipulate attributes of the actual plot line, and to modify the Workspace selection based on the entries included in a particular plot series.

Selecting a Series: The series available for the selected plot are listed at the top of the folder. To perform operations on a series, select the series in the list. Information for the selected series is displayed in the lower portion of the Series folder.

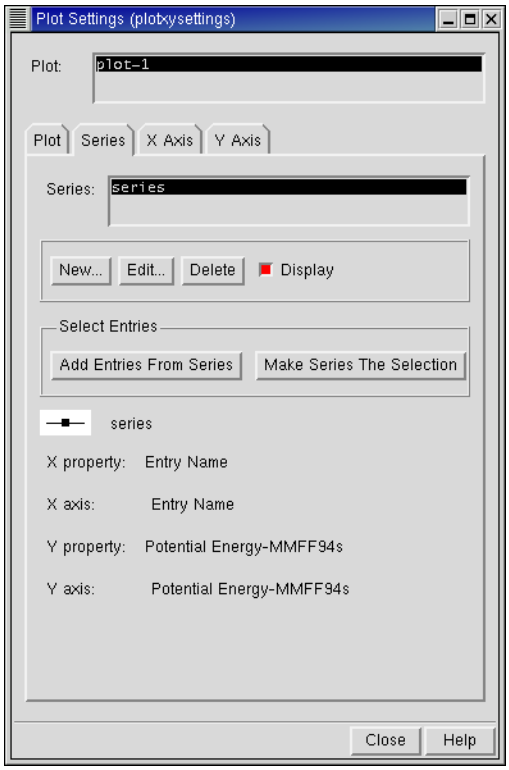


Figure 9.5. The* Series *folder of the* Plot Settings *panel.

Adding a Series: To add another data series to the selected plot, click New. The New Series dialog box is displayed. Select the desired values, and then click New to generate a plot line for the series. The controls are the same as in the New Plot dialog box—see Section 9.1 on page 119 for more information.

Editing an Existing Series: To change the settings for a series, click Edit. The Modify XY Data Series dialog box is displayed. Modify the settings and click Edit to implement your changes. The controls are the same as in the New Plot dialog box—see Section 9.1 on page 119 for more information. You can change all attributes of the series, including the name and the data to be displayed.

Deleting a Series: To delete the selected series click the Delete button.

Displaying or Undisplaying a Series: To display or undisplay the selected series, select or clear the Display button.

Adding Series Entries to the Project Table Selection: Click Add Entries From Series to add entries corresponding to the selected series to the entry selection in the Project Table.

Making a Series the Project Table Selection: To replace the entry selection in the Project Table with the entries corresponding to the selected series, click Make Series The Selection.

9.3.3 Changing X and Y Axis Display

The X Axis and Y Axis folders contain tools that allow you change the names, scales, and display status of the x- and y-axes, respectively. You can display more than one x-axis or y-axis on each plot.

Selecting an Axis: The X Axis and Y Axis lists display all of the axes that exist in the selected plot. You can select an axis from the list and change its characteristics. Information on the selected axis is displayed at the bottom of the folder.

Creating an Additional Axis: To generate additional axes for the selected plot, click the New button and set the controls in the dialog box that is displayed. Click New to generate the new axis.

Editing Axis Definitions: To edit the title, minimum and maximum values, and number of scale markers for the X and Y axes, click the Edit button, set the controls in the dialog box that is displayed and click Edit to implement your changes.

Deleting an Axis: To delete an X or Y axis, select the axis from list and click Delete.

Displaying and Undisplaying an Axis: To display or undisplay an X and Y axis, select the axis from the list select or clear the Display button.

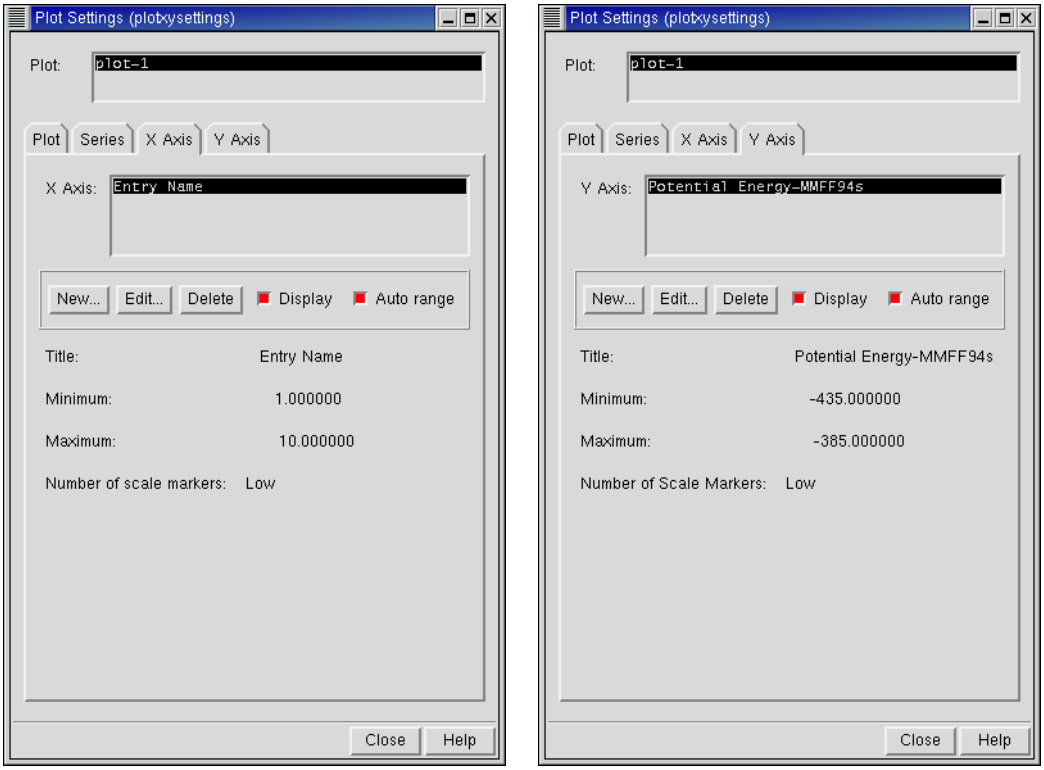


Figure 9.6. The X Axis ***and*** Y Axis ***folders of the*** Plot Settings ***panel.***

Setting the Axis Range: To set the axis range to the combined range of all the data series, select Auto range. To set the range manually, deselect Auto range, click Edit, and set the range.

9.4 Updating Plots to Reflect Project Table Changes

If the data values in the Project Table that are used for a plot have changed, you can update the plot with the new values by choosing Update Selected Plots from the Plot menu. For example, if you run a job with Replace selected, some cells in the table may acquire new values. If you want these values to replace old values in a plot, select the plot, then use the Update Selected Plots command.

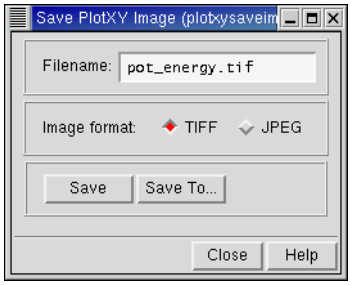


Figure 9.7. The Save PlotXY Image ***panel.***

9.5 Saving Plot Images

The Save PlotXY Image panel is used to save an image of the plotting panel to a file. To open the Save PlotXY Image panel, choose Save PlotXY Image from the Plot menu.

Saved images have the same dimensions in pixels as the Plot XY panel. For images to save properly, other windows must not overlap the Plot XY panel. Two image formats can be selected from the panel: TIFF and JPEG.

TIFF

When Maestro saves an image as a TIFF file, it uses no compression. This means that the image is “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. The JPEG file format specifies a means of compressing natural images that doesn't 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.

In Maestro, the JPEG Quality parameter is fixed at 75, and the most common JPEG file format, JPEG-File Interchange Format (JFIF), is used.

Surfaces

The Maestro surface facility allows you to create and visualize molecular structure surfaces, extended radius surfaces, van der Waals surfaces, and maps of active sites in receptor molecules; to import surfaces; and to display electrostatic potential surfaces, density surfaces, and molecular orbitals generated by Jaguar.

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*.

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 Surface Table panel. From this panel, you can change surface display properties, such as transparency, display style, and color.

10.1 Generating Surfaces

From the Surfaces submenu of the Display 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.

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.

10.1.1 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.

Name

You can name the surface by entering the name in the Name text box. If an entry has more than one surface, each surface name for that entry must be unique.

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 Select and using the Atom Selection dialog box. If you want to reset the atom selection, click Clear. If you have Show Markers selected, the atoms you select are marked in the Workspace.

Surface Context

The surface is actually generated for the atoms specified in the Surface context section, 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 10.4.1 on page 139 for details.

Image Quality

In the Molecular Surface panel you can set the quality of the image to Low, Medium, or High. These controls set the grid spacing for surface generation. The high quality surface is smoother but takes longer to generate. The van der Waals and extended radius surfaces do not use grids, so there is no corresponding image quality section.

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.

Create Surface

To start the molecular 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.

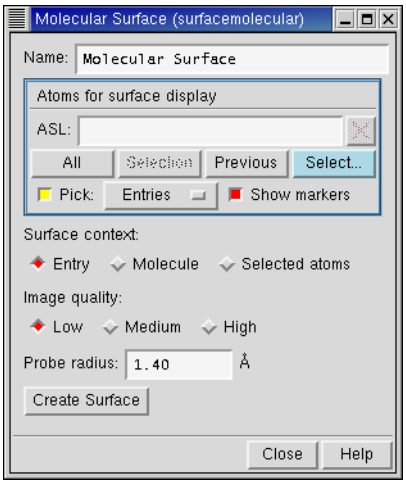


Figure 10.1. The Molecular Surface ***panel.***

10.1.2 Molecular Structure 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. Changing the solvent sphere or 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.

To open the Molecular Surface pane, choose Molecular Surface from the Surfaces submenu of the Display menu. Instructions for using the settings in the Molecular Surface panel are described in Section 10.1.1 on page 129.l

10.1.3 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.

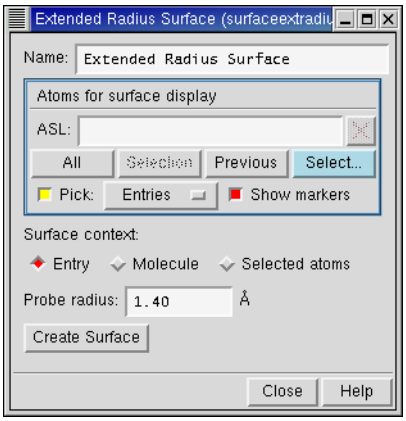


Figure 10.2. The Extended Radius Surface ***panel.***

To open the Extended Radius Surface panel, choose Extended Radius from the Surfaces submenu of the Display menu. Instructions for using the settings in the Extended Radius Surface panel are described in Section 10.1.1 on page 129.

10.1.4 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 van der Waals from the Surfaces submenu of the Display menu. Instructions for using the settings in the VDW Surface panel are described in Section 10.1.1 on page 129.

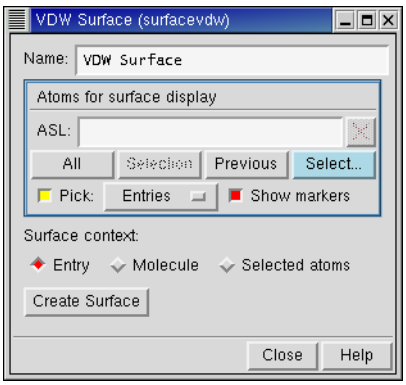


Figure 10.3. The VDW Surface ***panel.***

10.2 Sitemaps

SiteMap is a 3D graphics tool that is designed to help you to visualize the preferred locations of ligand atoms in a receptor site. Using the Sitemap panel, you can generate a surface that displays hydrophobic and hydrophilic regions within the active site of a protein. To open the Sitemap panel, choose Sitemap from the Surfaces submenu of the Display menu.

10.2.1 Background

Given a receptor structure, SiteMap partitions the accessible space in the active site into three types of regions:

1. **Hydrophobic**—regions that are favorable for occupancy by hydrophobic ligand groups
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, in contrast, 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

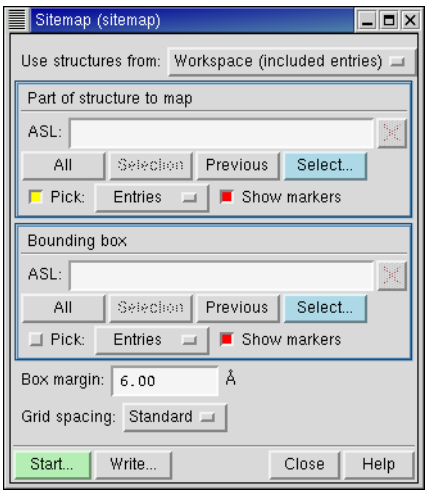


Figure 10.4. The** Sitemap **panel.

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). In SiteMap, 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, site maps depend on more than the character of the nearest receptor atom. Moreover, site maps explicitly show the shape and extent of hydrophilic and hydrophobic regions, something a receptor-surface display cannot do. The site maps behave rather like an "extraradius" surface in that the atoms of a stick figure representation of the ligand can approach but should not penetrate the site map surface (except in hydrogen bonding regions, where internuclear distances are expected to be smaller than normal contact van der Waals distances).

Hydrophilic Map: SiteMap constructs a measure of hydrophilicity 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 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 thus are taken to be 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 kcal mol^{-1}. The hydrophobic regions for human renin defined in this way are illustrated in the stereo pair shown in Figure 3 of Weber, Halgren et al., *J. Med. Chem.* **1991**, *34*, 2692-2701.

10.2.2 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 Å 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 Å, well depth 0.2 kcal mol^{-1}, and point dipole moment 2.3 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 kcal mol^{-1}) and displays the corresponding hydrophilic and hydrophobic volumes as surfaces.

10.2.3 Specifying a Structure to Be Mapped

To create a sitemap of a 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 Select to open the Atom Selection dialog box and select atoms. If Show Markers is selected, a dark pink trace is superimposed on the selected atoms and bonds.

To clear the atom selection, click Clear. Clearing the selection does not delete existing sitemaps.

10.2.4 Defining the Mapping Box

In addition to specifying the structure for which a sitemap 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 Show 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.

10.2.5 Running the Sitemap Job

In contrast to the generation of other types of surfaces, site mapping is run as a job. After you have configured the Sitemap 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. In the Start dialog box, enter a unique name for the job, enter your login and host (if they are different from the machine on which you are starting the job), and click Start to launch the job. The Monitor panel is displayed and the job's progress is printed to the window in the upper portion of the panel.

If the job finishes while it is being monitored, the results are automatically incorporated and the sitemap is displayed. If the job is not being monitored when it finishes, you can open the Monitor panel from the Applications menu in the main window and monitor the completed job to incorporate the results.

Once the sitemap for a particular entry has been generated, the surface information is incorporated into the Project Table and denoted in the Surf column for the entry with a button bearing the letter S. Click this button to open the Surface Table panel and view the data associated with this surface.

10.2.6 Viewing the Sitemap Surface

The sitemap is displayed as a pair of isosurfaces generated from the hydrophilic and hydrophobic grids. The default isovalues (–6 and –0.5 kcal/mol) can be changed in the Maestro 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.

10.3 Importing Surface or Volume Files

You can import Maestro `.vis` files or Jaguar `.plt` files, associate this data with a project entry, and display the data as a surface.

To import a file, choose Import from the Surfaces submenu of the Display menu, or click the Import button in the Surface Table panel. Browse for the desired `.plt` or `.vis` file and click Import. In the Choose Entry dialog box, choose the entry to which the surface or volume data belongs. 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 Surf column of the Project Table or by clicking the diamond in the V column of the surface table in the Surface Table panel.

Jaguar `.plt` 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.

A Maestro `.vis` file contains 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.

You can create `.plt` or `.vis` files using the Jaguar panel. When you run a plot job from the Jaguar panel, the surface and volume data is automatically incorporated into the project and displayed. See Section 4.12 of the *Jaguar User Manual* for details.

10.4 The Surface Table Panel

The Surface Table panel is used to import, modify, and view surfaces and their properties. To open the Surface Table panel, choose Surface Table from the Surfaces submenu of the Display menu.

The surfaces table contains all surfaces for all entries that are included in the Workspace (see Figure 10.5). Scratch entries are not part of a project and thus cannot be used.

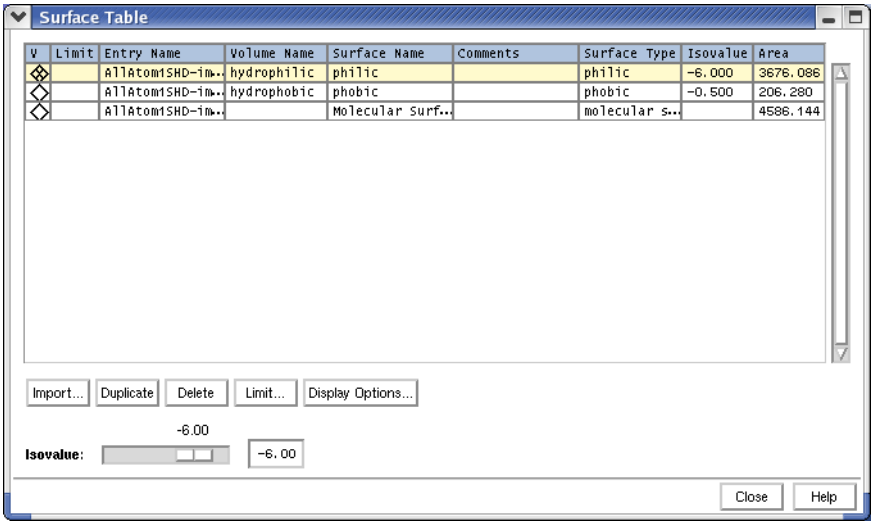


Figure 10.5. The Surface Table ***panel.***

The columns of the surface table are described in Table 10.1.

Table 10.1. Surface table columns.

Column	Purpose
V	Displays or undisplays 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 Name	Lists the name of the entry that contains the surface.
Volume Name	Lists the name of the volume from which the isosurface was created.
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 orbitals.
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).

To display a surface in the Workspace, click the diamond in the V (Visible) field for the desired surface.

To change the name of a surface, enter a new name in the Surface Name field.

At the bottom of the panel are buttons for importing, duplicating, deleting, and limiting surfaces, as well as controlling the display of surfaces. You can also adjust the isovalue of a volume with the slider or the text box. These controls and buttons are described in the following sections.

10.4.1 Importing, Modifying, and Deleting Surfaces

Importing Surfaces

To import a `.vis` or `.plt` file from the Surface Table panel, click Import, browse to select the desired surface file, and click Import. In the Choose Entry dialog box, select an entry with which to associate the imported data and click Choose. You can also import surfaces by choosing Import from the Surfaces submenu of the Display menu in the main window.

When you import a surface or volume file, 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.

Changing isovalues

The isovalue is the current value of the property that was used to create the surface. Surfaces generated by Jaguar and Sitemap 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 Isovalue text box at the bottom of the panel or use the slider to adjust the isovalue. The surface is redisplayed with the new isovalue.

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 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.

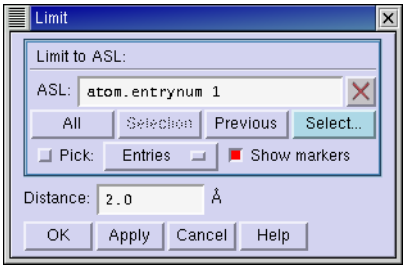


Figure 10.6. The Limit ***panel.***

Deleting surfaces

To delete a surface, select it in the surfaces table and click Delete.

10.4.2 Changing the Appearance of the Surface

You can adjust various characteristics of the surface's appearance using the controls in the Display Options panel.

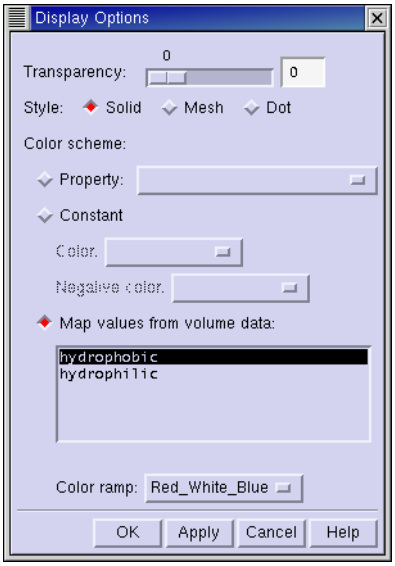


Figure 10.7. The Display Options ***panel.***

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 slider. Mesh and Dot surfaces are opaque unless the Transparency slider is set to 100%, when they become invisible.

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.
- Constant—the entire surface is colored with the same color, which you can choose from the Color option menu.

  When a surface has both positive and negative portions (as with orbitals), 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. The range of colors is determined by the range of values in the volume. 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. You can also create your own color ramp (see Appendix E for instructions).

Customizing Maestro

Many aspects of the Maestro interface can be customized. This chapter describes customizing the panel layout, the Maestro program preferences, the Workspace appearance and 3D viewing. Many of the changes described in this chapter can be saved explicitly, so that they are preserved in subsequent Maestro sessions. The changes are stored in the `$HOME/.schrodinger/maestro`*vv* directory, where *vv* is the two-digit Maestro version number (60 for this release). This directory is referred to hereafter as the *preferences* directory.

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 12.3 on page 159.

11.1 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), restore the panels you had open, and arrange the panels in a cascade, from upper right to lower left, by choosing the corresponding items from the Display menu.

You can save the size and location changes in a layout file, by choosing Save Panel Layout from the Maestro menu in the main window. Maestro immediately saves your panel settings to the file named `layout.res` in your preferences directory. 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 Saved Layout from the Maestro menu.

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.

11.2 Setting Preferences

The Maestro Preferences panel has seven folders, each of which contains controls for modifying Maestro's default behavior according to your personal preference. Changes made to interface 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 preferences directory.

To open the Preferences panel, choose Preferences from the Maestro menu.

11.2.1 Changing Font Size for Interface Component Text

The Font Size folder of the Preferences panel allows you to change the font size of the text that is displayed in the GUI. Changing the font size may change the amount of space each Maestro panel or window requires.

To select a new default font size, click Small, Medium, or Large. The actual point size depends on the size of your monitor screen. The default is Medium. After you have made your selection, restart Maestro to implement the change.

11.2.2 Setting Project Synchronization and Storage Preferences

The Project folder of the Preferences panel contains a number of options for saving modifications of a Workspace structure to the corresponding project entry, saving projects, and opening projects.

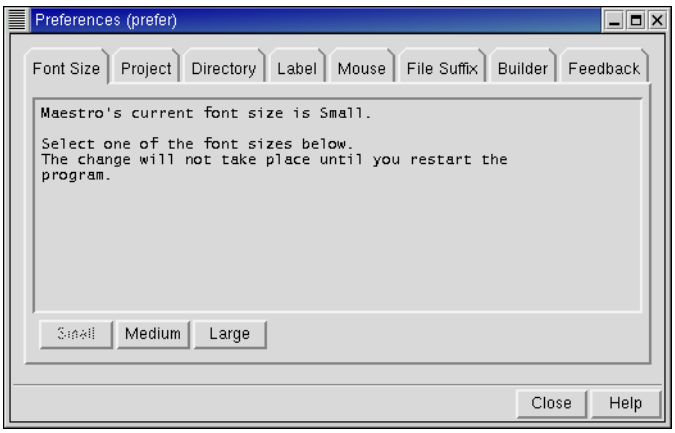


Figure 11.1. The Font Size ***folder of the*** Preferences ***panel.***

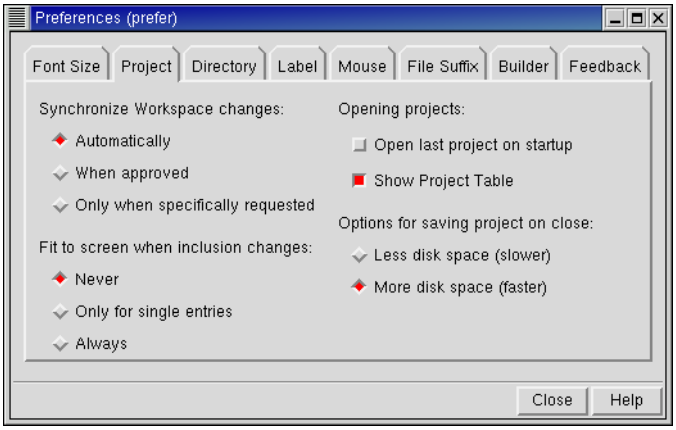


Figure 11.2. The Project ***folder of the*** Preferences ***panel.***

Synchronize 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 synchronization 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 synchronize, 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 exclamation point icon in the status bar to save any changes.

Fit to screen when inclusion changes

In this section you can set preferences for when an automatic fit-to-screen is performed. The action only applies when you include or exclude an entry from the Workspace. You can choose between Never, which turns off automatic fitting, Only for single entries, which performs a fit only when there is a single entry in the Workspace, and Always, which performs a fit whenever an entry is included or excluded.

Opening projects

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 by using the `-p` option. See Section 1.1 on page 1 for more information.

You can also choose to display the Project Table when you open a named project. This is the default behavior, but it does not apply to the scratch project.

Options for saving project on close

When you open a project, the initial state is stored in compressed format, and the working copy is stored in uncompressed format. When you close a project, the initial state is replaced with a compressed version of the current state of the project. You can choose to keep or to remove the uncompressed current state by selecting one of the following options:

- Less Disk Space (slower): The uncompressed version is removed. When you open the project again, the compressed initial state must be uncompressed before it is read. This option is useful if storage space is an issue.
- More disk space (faster): The uncompressed version is kept. When you open the project again, the uncompressed version is read.

Prior to the Maestro 5.1 release, projects were only stored in uncompressed format. When you open a project from a previous release, a copy of the project is compressed and stored as the initial state.

11.2.3 Specifying a Default Working Directory

The Maestro working directory is the directory to which file and project selectors open, and to which job files are written. The default initial working directory is the Maestro startup directory. By changing the settings in the Directory folder of the Preferences panel, you can specify a default working directory.

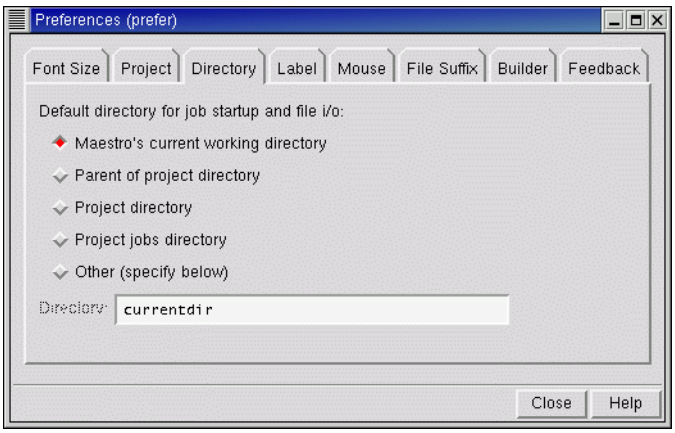


Figure 11.3. The Directory ***folder of the*** Preferences ***panel.***

In addition to the option Maestro's current working directory, you can choose from Project directory, Parent of project directory, Project jobs directory, and Other. If you choose any of the project-related options, the working directory is automatically updated when you begin working in a different project. If you choose Other, you must enter a directory in the Directory text box. The Other option may be useful if you keep all Maestro-related files in one area of your home directory.

If you change the working directory using the `cd` command in the command input area, the selection made in the Directory folder is superseded. However, if the selection is project-related, it is reapplied if you open a new project. If you use the filter in a file or project selector, the filter is retained until you change it or change the working directory.

11.2.4 Customizing Atom Label Appearance

The Label folder of the Preferences panel contains controls for defining the separator between properties in atom labels, the font, and the location of the label. You can also choose whether to display labels for hidden atoms, and display the property name in the label as well as the property. Changes made in the label preferences are immediately applied to existing labels.

- 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.
- Label Font: To change the font, choose a font style from this option menu.
- Field Separator: By default, the atom label fields are separated by a space. To add a separator such as a colon, semicolon, or vertical bar, type the character in this text box.

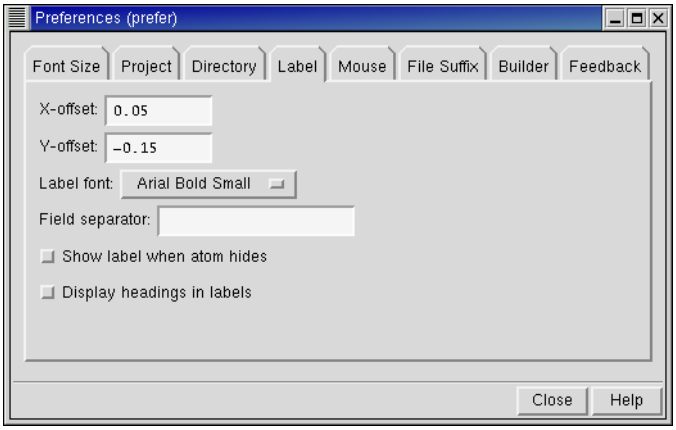


Figure 11.4. The* Label *folder of the* Preferences *panel.

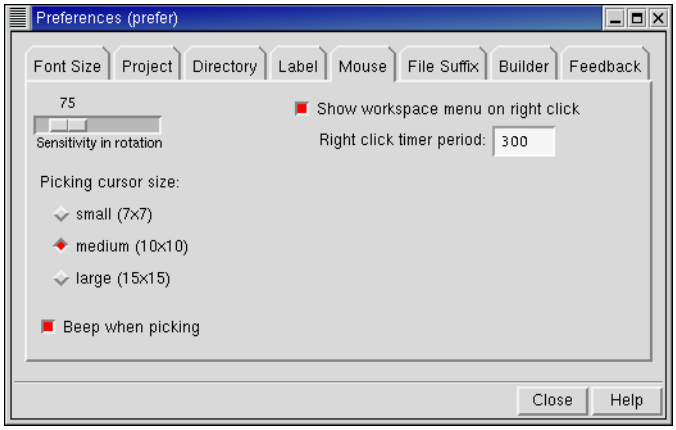


Figure 11.5. The Mouse ***folder of the*** Preferences ***panel.***

- Show label when atom hides: You can display labels for atoms that are hidden by selecting this option. 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.
- 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.

11.2.5 Setting Mouse Preferences

If you want to change the sensitivity of rotation of Workspace structures to mouse movement, use the Sensitivity in rotation slider in the Mouse folder to adjust the sensitivity. Increasing mouse sensitivity means that moving the mouse results in greater movement of the molecule in the Workspace.

You can select the picking cursor size by choosing small, medium or large.

You can choose whether or not audio feedback is given when you use the mouse to pick atoms in the Workspace. By default, Beep when picking is selected.

11.2.6 Setting File Suffix Preferences

You can change the default file suffixes that are used for the file types that Maestro recognizes in the File Suffix folder. These suffixes are appended to file names when you export structures from the Export panel. They do not include suffixes for file formats converted by Babel.

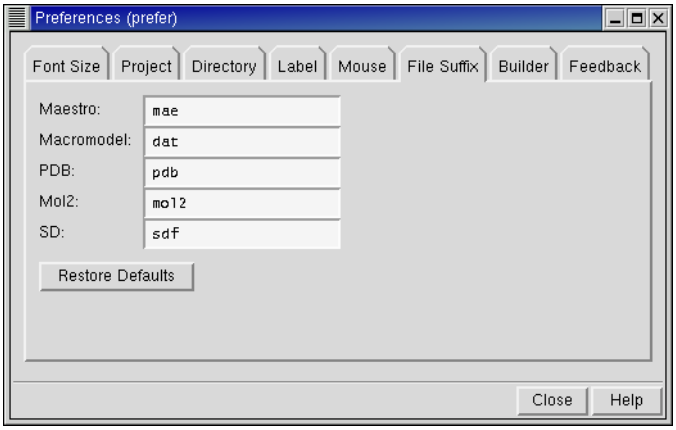


Figure 11.6. The File Suffix ***folder of the*** Preferences ***panel.***

11.2.7 Setting Builder Preferences

In the Builder folder 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.

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

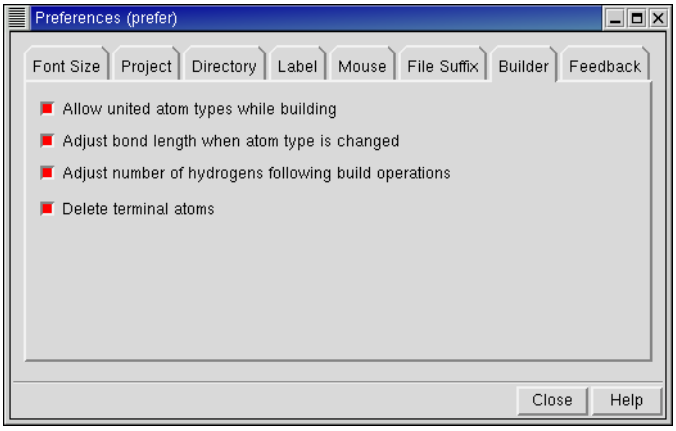


Figure 11.7. The Builder ***folder of the*** Preferences ***panel.***

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.

11.2.8 Setting Feedback Preferences

You can choose whether atom information is displayed in the status bar when the cursor pauses over an atom in the Workspace. If you select Show feedback, the status bar displays the following information about the atom:

```
chain:residue number :(element) PDB :charge:"userchoice"
```

`chain`	chain name
`residue`	residue name
`number`	residue number + insertion code
`element`	element
`PDB`	PDB atom name
`charge`	formal charge of the atom
`userchoice`	Entry Name or Title

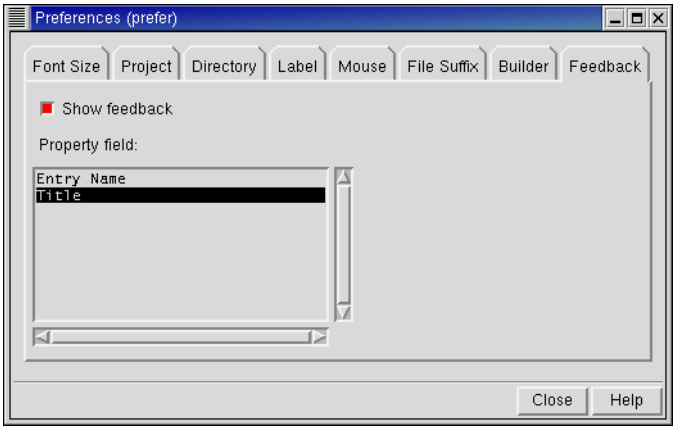


Figure 11.8. The Feedback ***folder of the*** Preferences ***panel.***

You can choose what is displayed in the `userchoice` field by selecting an item from the Property field list.

11.3 Changing the Workspace Appearance

You can adjust the appearance of the Workspace to fit the way you work best. You can hide or display many of the main window controls and change the background color of the main window.

11.3.1 Showing or Hiding Controls and Displays

The following five items in the Display menu hide or show main window controls and displays:

- Toolbar
- Clipping Planes Window
- Command Input Area
- Status Bar
- Sequence Viewer

You can also right-click on any of these items and choose Hide from the shortcut menu.

11.3.2 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. The background color can be retained for printing.

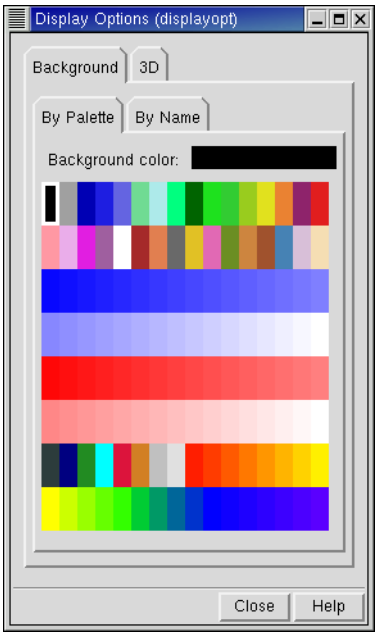


Figure 11.9. The Background ***folder of the*** Display Options ***panel.***

To change the background color, choose Display Options from the Display menu of the main window and select the Background folder. Choose a color in the By Palette subfolder, or select a color by name in the By Name subfolder. When a color is selected, a sample of the color is displayed in the Background color box.

11.4 Setting Up 3D Viewing

Maestro provides several tools to enhance viewing of complex structures. These tools include stereo viewing, perspective, fogging distant atoms, and depth cues and are described in the sections that follow.

11.4.1 Specifying a Stereo Viewing Method

Maestro's default stereo viewing method is wall-eyed. In this method of stereo viewing, the left eye looks at the left image, and the right eye looks at the right. The other option is cross-eyed viewing, in which the left eye looks at the right image and the right eye looks at the left.

Maestro also supports hardware stereo display. On both Linux and SGI platforms, stereo-in-a-window is supported, and full-screen stereo is supported on SGI platforms. For details, see the *Schrödinger Product Installation Guide*.

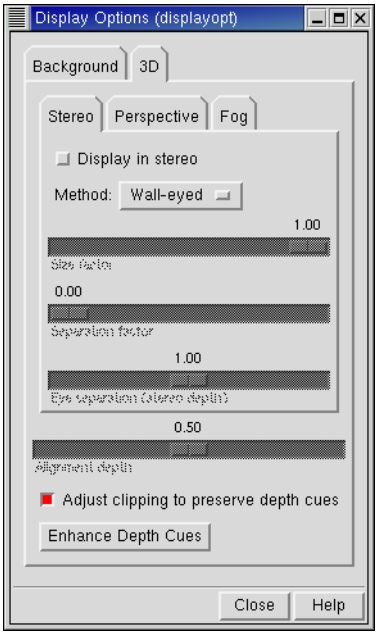


Figure 11.10. The Stereo ***folder of the*** Display Options ***panel.***

To set the stereo viewing options, choose Display Options from the Display menu in the main window and select the Stereo subfolder of the 3D folder. To select a stereo viewing method, choose Wall-eyed, Cross-eyed or Hardware from the Method option menu. To view the Workspace in stereo, select Display in 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.

11.4.2 Enabling Perspective

Maestro's Perspective feature enhances 3D graphical representation by scaling items in the Workspace in proportion to their distance from the viewing plane ("camera").

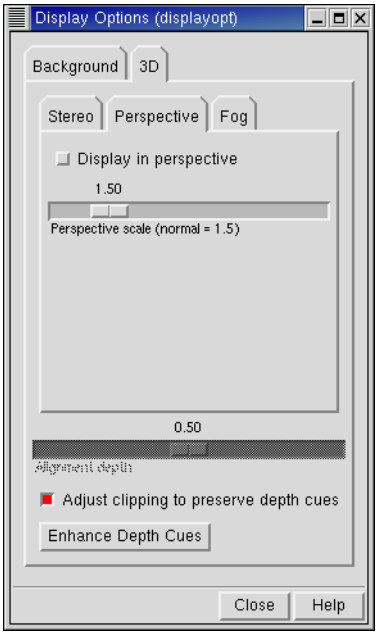


Figure 11.11. The Perspective ***folder of the*** Display Options ***panel.***

The perspective controls are in the Perspective subfolder of the 3D folder. You can adjust the scaling using the Perspective scale slider. The green lines in the Top View window move to reflect the viewing volume available at a given value on the Perspective scale.

11.4.3 Enabling Fog

Maestro's Fog feature causes atom colors in the displayed structure to 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.

The fog controls are in the Fog subfolder of the 3D folder. Fogging is turned off by default. To enable fogging, select On or Automatic from the Display fog option menu. 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*. You can independently apply fogging to atom labels using the Display fog on atom labels option. You can also turn fogging on or off with the Set fog display state button menu in the main toolbar.

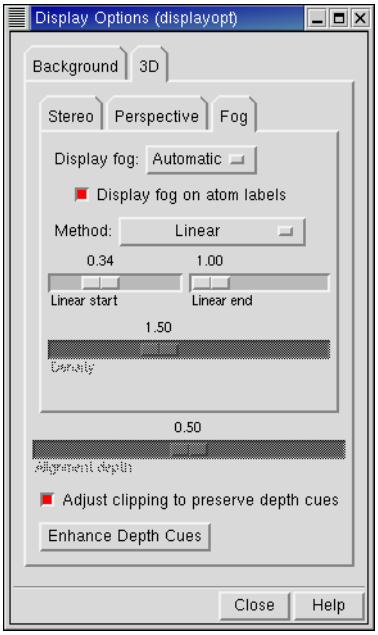


Figure 11.12. The Fog ***folder of the*** Display Options ***panel.***

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 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.

11.4.4 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 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 folder, or click the Enhance depth cues button in the main toolbar.

Scripting in Maestro

Maestro provides several facilities for creating scripts. You can generate scripts using Python or 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.

12.1 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.

To install a Python script, choose Manage from the Scripts menu to open the Manage Scripts panel (see Figure 12.2), then click Install Scripts to open the Install Scripts panel (see below). You can install the scripts that came with the distribution or browse to the directory containing your own scripts. Click a box in the Install column to select a script. The script's 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 in the Scripts menu. Click OK to add the script to

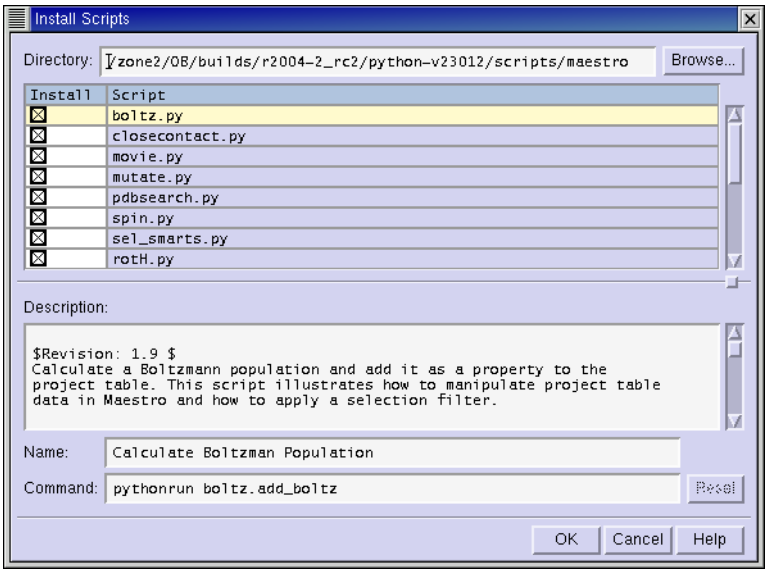


Figure 12.1. The Install Scripts ***panel.***

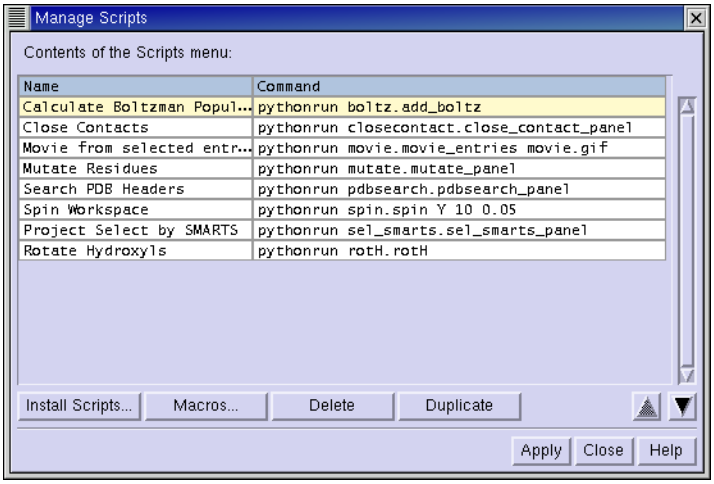


Figure 12.2. The Manage Scripts ***panel.***

the menu and close the panel. If the script already exists in the menu, you are asked if you want to overwrite it.

Note: The Install Scripts panel only displays files with a `.py` suffix, the standard suffix for Python scripts.

To install a macro from the Manage Scripts panel (see Figure 12.2), click Macros to open the Macros panel, select a macro from the list, and click Install.

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 using 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.

12.2 Customization Using 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.

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. 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 12.1 on page 157.

For more information on using Python with Maestro, see the Python Tutorial:

`$SCHRODINGER/docs/python/tutorial/py23_tutorial/`

12.3 Customization 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 Command Script Editor from the Edit menu.

12.3.1 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 12.3). 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.

You can control which types of commands are displayed by using the Show/Hide Commands panel (see Figure 12.4). To open this panel, click Show/Hide in the Command Script Editor panel. If a command is not logged, open the relevant folder and select the button corresponding to the command, click Rebuild Command History, and then click Close. The command of interest should now appear in the list.

12.3.2 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. Individual commands can be selected or deselected by clicking. A group of commands can be selected 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.

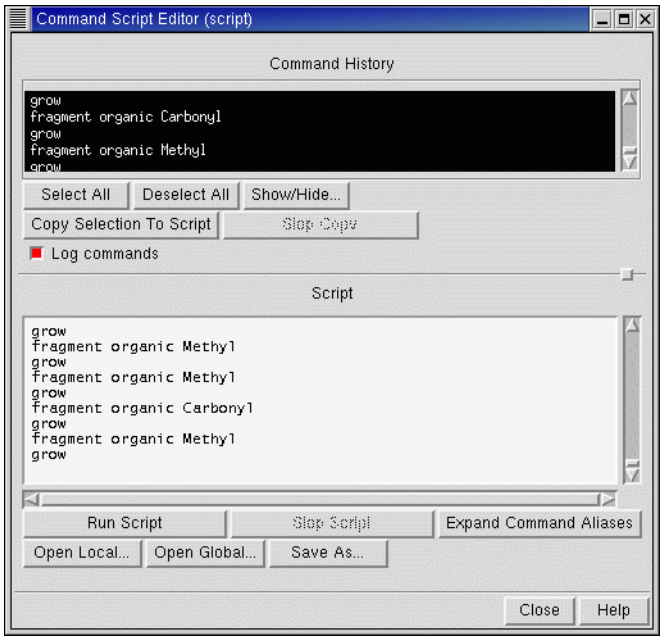


Figure 12.3. The Command Script Editor ***panel.***

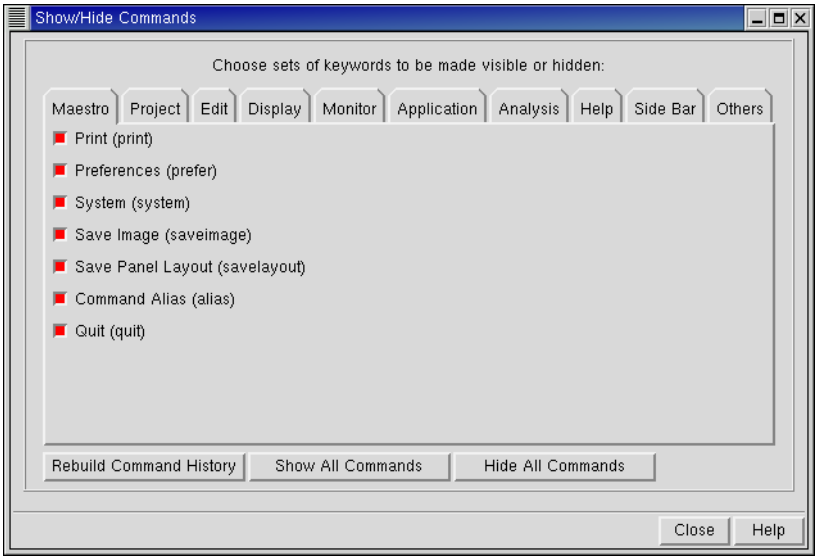


Figure 12.4. The Show/Hide Commands ***panel.***

Once you have selected the desired commands, copy them to the Script text area by clicking Copy Selection To Script. Copying many commands may take some time. To interrupt the copying process, click Stop Copy. This button is only active during a copy operation.

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.

12.3.3 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.

12.3.4 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 `$SCHRODINGER/maestro-v`*version*`/data/res` directory

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.

12.3.5 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.

To halt the execution of a script, click Stop Script.

12.3.6 Customizations You Can Perform With a Script

As mentioned above, 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 Display Options from the Display menu of the main window.
2. Click the Background tab.
3. Choose a color in the By Palette folder, or select a color name in the By Name folder.

To specify a stereo viewing method:

1. Choose Display Options from the Display menu of the main window.
2. In the 3D folder, click the Stereo tab.
3. Choose a stereo display technique from the Method option menu.
4. Adjust the Size Factor and Scale Factor if necessary.

To enable perspective:

1. Choose Display Options from the Display menu of the main window.
2. In the 3D folder, click the Perspective tab.
3. Adjust the Perspective Scale, if needed.

To hide the toolbar:

- Choose Toolbar from the Display menu of 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 toolbar
```

To hide the command input area:

- Choose Command Input Area from the Display menu of 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 Clipping Planes Window from the Display menu of 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
```

12.4 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 Command Aliases from the Maestro menu.

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 any subsequent Maestro session. 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.

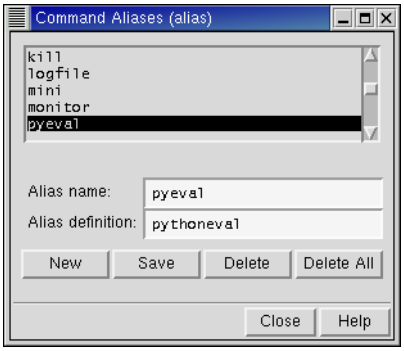


Figure 12.5. The** Command Aliases **panel.

12.5 Creating Macros

Maestro allows you to create two kinds of macros: named macros and function key macros.

12.5.1 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 Macros from the Edit menu.

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 12.1 on page 157.

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 Command Input Area from the Display menu.

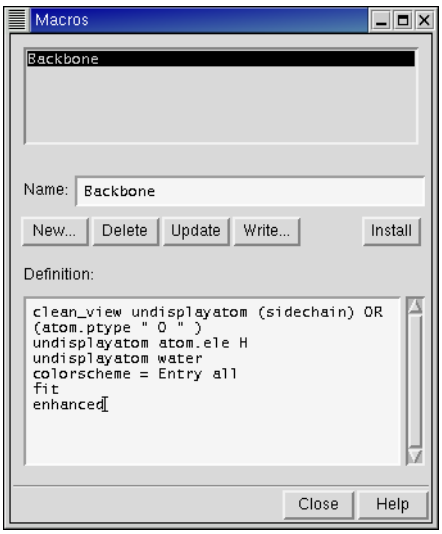


Figure 12.6. The Macros ***panel.***

Figure 12.7. The Function Key Macros ***panel.***

12.5.2 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 (F1-F12).

To open the Function Key Macros panel, choose Function Key Macros from the Edit menu.

To assign a macro to a function key, select the key from the Macro Key option menu, 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.

Printing and Saving Workspace Images

In addition to creating Maestro, MacroModel, PDB, Sybyl Mol2, and MDL SD structure files, Maestro can produce high-quality print and electronic representations of structures depicted in the Workspace. You can use the tools in the Print panel to generate PostScript and Encapsulated PostScript files, and use the Save Image panel to create TIFF and JPEG images. For information on writing (exporting) structure files, see Chapter 2.

13.1 Printing an Image (File or Printer)

From the Print panel, you can print or create PostScript or Encapsulated PostScript images of structures currently rendered in the Workspace. To open the Print panel, choose Print from the Maestro menu. The settings available in the Print panel are described below.

Print To

To print an image, select Printer. To write a PostScript (PS) or encapsulated PostScript (EPS) file, select File.

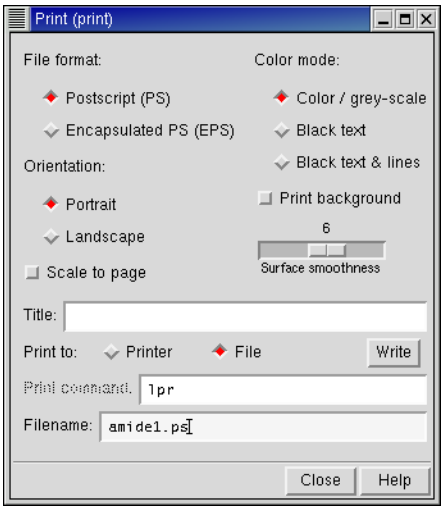


Figure 13.1. The* Print *panel.

File Format

If you selected Printer in the Print To section, only the Postscript (PS) option is available, because you cannot directly print encapsulated postscript. If you selected File, select Postscript (PS) or Encapsulated PS (EPS).

Orientation

Select Portrait or Landscape to determine the orientation of the image.

Scale To Page

Select Scale to Page to reduce or enlarge the image to occupy the available space on a standard page. When Scale to Page is not selected, the image is printed roughly the same size as it appears on screen.

Color Mode

The Color Mode selections are Color/Grey-scale, Black Text, and Black Text & Lines. Selecting the Color/Grey-scale option allows you to print or save images exactly as they appear on screen. If atom labels and other text appears in color, they are printed in color. It can be difficult to read atom labels and other text in color. To force atom labels and any other text to print in black, select Black Text. To force text plus any lines, such as markers and wire frame bonds, to print in black, select Black Text & Lines. If you print to a black-and-white printer, the images are printed in grey scale instead of color.

Print Background

This button controls the printing of the background color of the Workspace. It is not selected by default because printing a background requires more ink (or toner) and time, and the default background color of the Workspace is black.

Surface Smoothness

Increasing the surface smoothness for an image helps to remove “blocky” edges on curved surfaces in your structure. However, there is a trade-off between degree of smoothing and amount of print time required. Particularly with small curved surfaces, the minute improvement in image clarity obtained from increasing the smoothness factor may not justify the increased time it takes to print the image.

To change the surface smoothing, drag the Surface Smoothness slider.

Title

You can enter a title in the Title text box. The title is printed in black text in the lower left corner of the page.

Print Command

If the UNIX shell you use requires a different print command from the default given in the Print Command text box, change the command in the text box to the required command.

When printing an image, Maestro creates a temporary PostScript file then prints this file using the specified command. If your printer requires the `lp` command instead of `lpr`, use the `-c` option to ensure that the temporary copy of the file to be printed is preserved until printing is complete.

Filename

If you are saving an image to a file, enter the file name in the Filename text box, including either the `.ps` or the `.eps` file extension.

13.2 Creating TIFF and JPEG Image Files

You can save electronic images of structures rendered in the Workspace in TIFF or JPEG format using the Save Image panel. To open the Save Image panel, choose Save Image from the Maestro menu.

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 Clipping Planes from the Display menu.
- Make sure there are no panels or dialog boxes overlapping the Workspace. This includes the Save Image panel.
- Make sure the cursor is not in the Workspace.

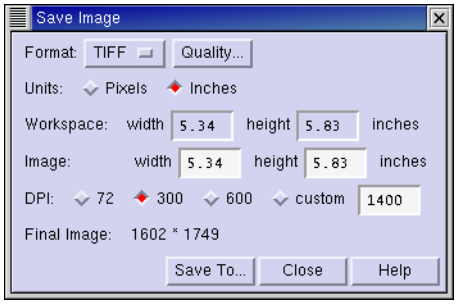


Figure 13.2. The Save Image ***panel.***

The Save Image panel allows you to set the following options:

- Format—choose Tiff or JPEG:
  - TIFF is an acronym for "Tag(ged) Image File Format", a file structure that allows pixel data to be stored in a variety of different internal formats. Format parameters such as byte order, image dimensions, and compression method are specified in labeled variables, or "Tags", which can either be placed within the file header or distributed throughout the file. When Maestro saves an image as a TIFF file, it uses no compression. This means that the image is "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 stands for "Joint Photographic Experts Group". JPEG is actually a compression method, not an image 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 to a human observer. 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, nevertheless, provided because it allows Maestro users to create extremely compact screen shots for sending with an e-mail message or inserting in web pages. Maestro uses the JPEG-based JPEG-File Interchange Format (JFIF), the most commonly used JPEG file format.

  Both TIFF and JPEG files can be imported into image manipulation programs.

- Quality—open the Image Quality dialog box, which allows you to adjust the quality of the image:
  - Smooth—Select this option to turn on scene anti-aliasing. This creates smoother edges, but takes longer to save the image.
  - Quality—(for JPEG only) Use the slider to select a quality level from 1 to 100. The default is 75. The higher the quality level, the longer it takes to save the image. For large resolution images, this can take awhile.
- Units—Choose pixels or inches. This choice determines the Workspace and Image units (see below).
- 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. To change the units, select either Pixels or Inches under Units .

- 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 under Units.
- 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.
- Final Image—Displays the final resolution of the image (in pixels). This value is not editable, but you can change it by changing the options above.

To save an image:

1. Choose TIFF or JPEG from the Format option menu.
2. If you want to increase the quality of the image:
   a. Click Quality to choose Smooth.
   b. For JPEG files, use the 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. Click Save To, navigate to a directory, and select or enter a file name.
7. Click Save.

Note: When saving high resolution images in wire or Ball & Stick molecular representation, you may need to adjust the wire width so the bonds remain visible at the higher resolution. This may take some experimentation, depending on the purpose of the image. See Section 5.2.3 on page 68 for information on changing the molecular representation attributes.

Job Control

Most computational jobs launched from Maestro are run under Schrödinger's job control facility. The job control facility provides a uniform mechanism for launching, monitoring and controlling calculations, both for jobs launched from Maestro and for jobs launched from the command line. The job control facility keeps information on jobs in a database that is set up for each user.

By default, the job control facility allows you to run jobs locally. However, you can also run remote and, in some cases, distributed jobs and parallel jobs. To run jobs run on a remote host, you must first configure job control by editing your `schrodinger.hosts` file, and setting up any protocol needed to connect to the remote host.

14.1 Configuring Job Control

Configuration of job control is done in the `schrodinger.hosts` file. The default installation of this file is configured to allow running of jobs locally, and no action is required by the user. However, if you wish to run distributed jobs, run jobs remotely, change the location of the scratch directory, or set up the remote environment, then job control must be configured. The following sections describe how to specify the scratch directory, how to prepare your account for remote job submissions, and how to modify the hosts file, `schrodinger.hosts`.

Information on configuring job control is also contained in the *Schrödinger Product Installation Guide*, including configuration of batch queues.

14.1.1 The Scratch Directory

Most jobs now run in a scratch directory by default, rather than in the directory from which the job was started. When a scratch directory is used, output and log files are created there and are copied back to the output directory when the job finishes, or when the job is being monitored in Maestro.

When a scratch directory is created automatically, it is named *tmpdir*/*username*/*unique_name*. The *unique_name* is usually the job name, but it can also have a sequence number appended to it in order to make the directory name unique.

There are a number of ways to specify the *tmpdir* directory. The job control facility uses the first specification found from the following list:

- The directory given on the command line with the `-TMPDIR` option. For example,

  `$SCHRODINGER/bmin -TMPDIR /scr/mmod_tmp` *job_name*

- The directory specified by the `SCHRODINGER_TMPDIR` environment variable, if this is set on the machine on which the job is started. To set this environment variable, execute the following command or add it to your shell startup script.

csh/tcsh: `setenv SCHRODINGER_TMPDIR` *scratch-directory*

bash/ksh: `export SCHRODINGER_TMPDIR=`*scratch-directory*

- The directory specified by the `tmpdir` setting for the host entry in the host database file, `schrodinger.hosts`.

For remote jobs, the following locations are also considered, if none of the above specifications is found:

- The directory specified by the environment variable `SCHRODINGER_TMPDIR` on the remote machine.
- The directory specified by the environment variable `TMPDIR` on the remote machine.

If no other specification for *tmpdir* is found, the directory `$HOME/.schrodinger/tmp` is used. In this case, the *username* is not used to form the scratch directory name, since it would be redundant.

Environment variables on the remote machine are created in the normal manner for a remote shell command. Note that environment variables are *not* created if the user's default shell is ksh. In all cases, *tmpdir* is created if necessary.

When the job finishes, the scratch directory is automatically removed, if the following conditions are met:

- The output files were all successfully copied back to the startup directory.
- The directory did not exist before the job started.

14.1.2 Preparing for Remote Job Submission

To run remote or distributed jobs, executing remote commands using the `rsh` or `ssh` command without specifying a password must be enabled. This typically requires one of the following:

- A `hosts.equiv` file exists in the `/etc` directory on each host. This file should contain a list of hosts amongst which users can log in without giving their passwords (provided that their userids are the same on each of the machines). Creating a `hosts.equiv` file usually requires root permission.

- A `.rhosts` file exists in the user's home directory on each of the remote hosts. The `.rhosts` file should list the names of the hosts and user name from which the user can log in without specifying a password. The list should contain two lines for each machine—one with the machine name alone and one with the fully qualified name:

  machine username
  machine.domain username

  The user name in the `.rhosts` file is optional if it is the same on the remote hosts. You do not need root permission to configure this file, but you must make sure that the file does not have "group" or "other" write permission.

Once you have configured `hosts.equiv` or `.rhosts`, use the following command to check for successful communication between the host that the job will be started on and each of the other hosts that the job will use.

```
rsh -l username machine date
```

This command should print the date from the host *machine*.

If you have a `schrodinger.hosts` file, you can automatically check all of the machines listed in it using the command

```
$SCHRODINGER/hunt -rtest
```

See the next section for more information about this command.

By default, the `rsh` and `rcp` commands are used for remote connection and copying. To use `ssh` and `scp` instead, set the environment variables `SCHRODINGER_RSH` and `SCHRODINGER_RCP` to `ssh` and `scp`.

14.1.3 The schrodinger.hosts File

The job control facility obtains information about the computers (hosts) on which it will run jobs from the `schrodinger.hosts` file. The hosts database file used for a given job is the first one found in the following list:

1. The file specified by the environment variable `SCHRODINGER_HOSTS`
2. The `schrodinger.hosts` file in the current directory
3. The `schrodinger.hosts` file in `$HOME/.schrodinger`
4. The `schrodinger.hosts` file in `$SCHRODINGER`

For distributed MacroModel jobs the following locations are searched first:

1. A file specified by the command line argument `-HOSTFILE`.
2. The file *jobname*`.hst` in the startup directory on the startup host, where *jobname* is the stem of the command file name for the current calculation (e.g., if the command file were called `cal_en1.com`, this file would be called `cal_en1.hst`).

The `schrodinger.hosts` file can be tested using the command:

```
$SCHRODINGER/hunt -rtest
```

This command tests the first `schrodinger.hosts` file found in the list above, excluding the one specified by `-HOSTFILE`. This command also attempts to contact each of the hosts listed, and thus also serves as a check on host accessibility and on whether `rsh` has been set up appropriately on the various hosts.

A sample `schrodinger.hosts` file is shown below.

```
# Schrodinger hosts file
#
name:         localhost
schrodinger: /software/schrodinger
#
name:         ahost
#
name:         bhost
#
name:         old_bhost
host:         bhost
schrodinger: /software/schrodinger_old
#
name:         another_host
processors:   2
tmpdir:       /scr
schrodinger: /usr/bin/share/schrodinger
#
# End of Schrodinger hosts file
```

The hosts file consists of one or more entries, each of which describes a host on which jobs can be run. There is usually a single entry for each machine on which you want to run jobs. For each entry in the `schrodinger.hosts` file, the following settings can be made:

`name:` *entry-label*
`host:` *machine-name*
`user:` *username*
`tmpdir:` *tempdir*

`processors:` *number of processors*
`schrodinger:` *installation-path*
`env:` *environment variable assignment*

The settings are described in the following sections. A full list of settings, including settings for batch queue configuration, is given in the *Schrödinger Product Installation Guide*.

The settings can be formatted with any combination of spaces and tabs, but the entire setting must be on one line. Any number of comments can be included in the file. Comments should start with a hash sign (#).

If you have installed Schrödinger products on multiple hosts, you may need to edit the `schrodinger.hosts` file on each host to add entries for the other hosts.

The `name` and `host` Settings

The `name` setting must be the first line for each entry. This is the name that is displayed in the list of known hosts in the menus of the product panels. Usually, *entry-label* is the name of a machine (a host) that can be used to run a calculation, but if it is not, you must include a `host` setting that supplies the host name. The `host` setting is only needed if the name line does not give the host address. You might, for example, want to provide an alias in the `name` setting and define the host name in a `host` setting if the host name is long. Another use of multiple entries for a single host is to specify different settings on a host, such as different scratch directories or different software installations. You can also use the `name` and `host` settings to specify a batch queue name and the host on which the batch system is available.

The host name does not need to include the full Internet address unless the host on which you plan to run (the execution host) is not on the same local network as the host from which you plan to submit jobs (the submission host).

The value `localhost` is a special `name` setting that means the host from which the job was submitted. In addition to this function, the `localhost` entry sets the default values of settings for all other entries. In the `schrodinger.hosts` file example above, the host entries `ahost` and `bhost` inherit the `schrodinger` setting from the `localhost` entry.

The `user` Setting

If you have different user names on the submission and execution hosts, you must include a `user` setting for the execution host in the `schrodinger.hosts` file on the submission host.

The `tmpdir` Setting

The `tmpdir` setting specifies a directory where scratch directories can be created, such as `/scr` or `/temp`. See Section 14.1.1 on page 173 for more information on scratch or temporary directories.

You can override the `tmpdir` setting in the `schrodinger.hosts` file by setting the `SCHRODINGER_TMPDIR` environment variable. For example, if the directory designated by `tmpdir` becomes full with files that you don't have permission to delete, you can set `SCHRODINGER_TMPDIR` to a different directory and continue to run Jaguar jobs.

The `processors` Setting

For stand-alone computers with multiple processors, set `processors` to the number of processors in the computer. For computer clusters, set `processors` for each node to the *total* number of processors in the entire cluster.

The `schrodinger` Setting

The `schrodinger` setting specifies the directory in which your Schrödinger software is installed on this host. This setting allows you to choose between versions of our software to use on the remote machine, if more than one version is installed. The `schrodinger` setting is also useful if your default shell (e.g. ksh) does not set the `SCHRODINGER` environment variable on remote machines when using `rsh` or `ssh`. You can provide multiple `schrodinger` settings for a single host entry.

You can override the `schrodinger` setting with the `-VER` and `-REL` options if you run a program from the command line. See Section 14.6 on page 188 for details.

The `env` Setting

The `env` setting specifies an environment variable that is to be set on this host when any job is started. The syntax of the setting is "*variable=value*", where *variable* is the environment variable and *value* is its value. For example,

```
env: SCHRODINGER_THIRDPARTY=/software/databases
```

To set multiple environment variables, include one `env` setting for each variable.

14.1.4 Software Version Selection

When a job is started on a local host, the job control facility compiles a list of software versions that are available on the host, and selects the first compatible version on the list. The list is compiled by combining lists from the following sources in the order given:

1. Software in the directory specified by $`SCHRODINGER`
2. Software in the directory specified by the `schrodinger` settings in the `localhost` entry and the entry for the host in `schrodinger.hosts`

The list from each source is sorted by architecture and release version before it is combined with the other lists. This list can be displayed by entering the command for the program with the `-LIST` option in a terminal window. If you are running a job from the command line, you can filter this list to select a version, a release, and an architecture. See Section 14.6 on page 188 for more information.

The version that is selected is not always the most recent, nor is it always the version specified for the host in the host entry in `schrodinger.hosts`. The way in which the list is ordered results in the following selections.

- If the most recent version is for an older architecture (e.g. MIPS-3 when MIPS-4 is also available), the most recent version for the newer architecture is selected.
- If the version found in the directory specified by the `schrodinger` settings for `localhost` is more recent than the version found for the host entry, the `localhost` version is selected.
- If the version found in the directory specified by `$SCHRODINGER` is older than the version found in any of the directories specified in the `schrodinger.hosts file`, the `$SCHRODINGER` version is selected.

When a job is started on a remote host (the *execution* host), the startup script for the program is run on the local host (the *submission* host), and is selected from the versions available on the local host as described above. On the execution host, a list is compiled, sorted as described above, combining lists from the following sources in the order given:

1. Software in the same directory as the startup script on the submission host.
2. Software in the directory specified by the `schrodinger` settings in the `localhost` entry and the entry for the host in `schrodinger.hosts` on the submission host.
3. Software in the directory specified by `$SCHRODINGER` on the execution host.

14.1.5 Environment Variables

The environment variables that can be used to control the execution of jobs are given in Table 14.1 on page 180. These environment variables are passed in the following order of precedence:

1. Environment variables exported explicitly by the program startup script.
2. Environment variables specified in the `schrodinger.hosts` entry.
3. Automatically exported environment variables.
4. Environment variables defined in the remote shell startup script file (for non-Korn shell users).

Table 14.1. Environment variables for controlling execution of jobs on remote hosts.

Variable	Purpose
SCHROD_LICENSE_FILE	Specify the license file to use if the license file is not installed in $SCHRODINGER.
SCHRODINGER_JOB_DEBUG	Control debugging output. Allowed values are: 0 No debugging output 1 Standard debugging output (same as entering -DEBUG from the command line) 2 Detailed debugging output (same as entering -DDEBUG from the command line)
SCHRODINGER_JOB_DISPOSITION	Specify how to incorporate job results into the project (same as entering -DISP from the command line) Available values are: append add entries to project replace replace project entries with new entries ignore do not incorporate entries Default: ignore
SCHRODINGER_JOBDB	Specify the full path name for the job database Default: ~/.schrodinger/.jobdb
SCHRODINGER_JOBDB_CLEANUP	Specify how long the completed job record is kept in the job database before being automatically deleted. For example, one day can be expressed as 86400, 1440m, 24h, or 1d.
SCHRODINGER_PROJECT	Specify the path name of the Maestro project into which the results of the job should be incorporated (same as entering -PROJ from the command line)
SCHRODINGER_RCP	Specify the command to use for remote copying. You can use rcp or scp, if they are specified in your path, otherwise you must use the full path name to the command.
SCHRODINGER_RSH	Specify the command to use for remote connection. You can use rsh or ssh, if they are specified in your path, otherwise you must use the full path name to the command.
SCHRODINGER_TMPDIR	Specify the full path name for the directory in which runtime temporary job directories are created. Overrides the tmpdir setting specified in the schrodinger.hosts file.

14.2 Starting Jobs

Once you have set all the options for a computational job using an application panel (e.g. the Current Energy panel in MacroModel), then you need to set the job options using the Start dialog box.

To open the Start dialog box, click the Start button on the panel. Then you can set the options for the job. These options vary, depending on the product you are using and some products have custom options for specific job types. For more details, see your product user manual. The basic options include the following:

Output

- Incorporate—Choose whether the new entries are appended to the Project Table, replace the existing entries, or are not incorporated into the Project Table at all. See Section 14.7 on page 191 for more information on incorporating output.

Job

- Name—Enter a name for the computational job. This name is used as a prefix for all files created during the calculation.

  Note: Maestro does *not* automatically assign new names to jobs or files. If files of the same name exist, a warning is displayed before any files are overwritten.

- Host—Choose a host, if you want to run the job on a remote machine. This option menu displays all the hosts defined in the `$SCHRODINGER/schrodinger.hosts` file, with the number of processors on the host in parentheses.
- Username—Enter your user name, if it is required for running the job on remote machines. The default value is the user name of the user who started Maestro. If this user name is not correct for the selected host, you can change it in this text box.
- CPUs—Specify the number of CPUs to use to run the job.

Once you have finished setting these options, you can click Start to start the computational job.

14.3 Monitoring Jobs

When a computational job is started, Maestro immediately goes into monitoring mode. The Monitor panel opens, and the log file for the job is displayed in the text area at the top of the panel. The display is updated as the log file changes. For some kinds of jobs, such as MacroModel and Jaguar geometry optimizations, the Workspace is updated with each new geometry as it is generated.

Note: If the job directory (the directory containing the input and output files for the job) is not mounted on the job execution host, the job can not be monitored in the Monitor panel or by `jobcontrol -view jobid` (issued at the command line).

Most Maestro operations stop the monitoring of a job. You can also exit monitoring mode by clicking Detach on the Monitor panel. You can resume or begin monitoring a job at any time by selecting it from the list of jobs in the Monitor panel.

You can monitor any job that uses Schrödinger software from the Monitor panel. The job control facility keeps a database of all your jobs on all hosts, regardless of whether they were initiated from Maestro or from the command line.

If you want to monitor a job and the Monitor panel is not open, choose Monitor Jobs from the Applications menu.

Every job proceeds through a series of well-defined stages. The current stage of a job is displayed as the job's Status in the Monitor panel. The Status of a completed job indicates the conditions under which it stopped. The job status descriptors that can appear in the Monitor panel are listed in Table 14.2.

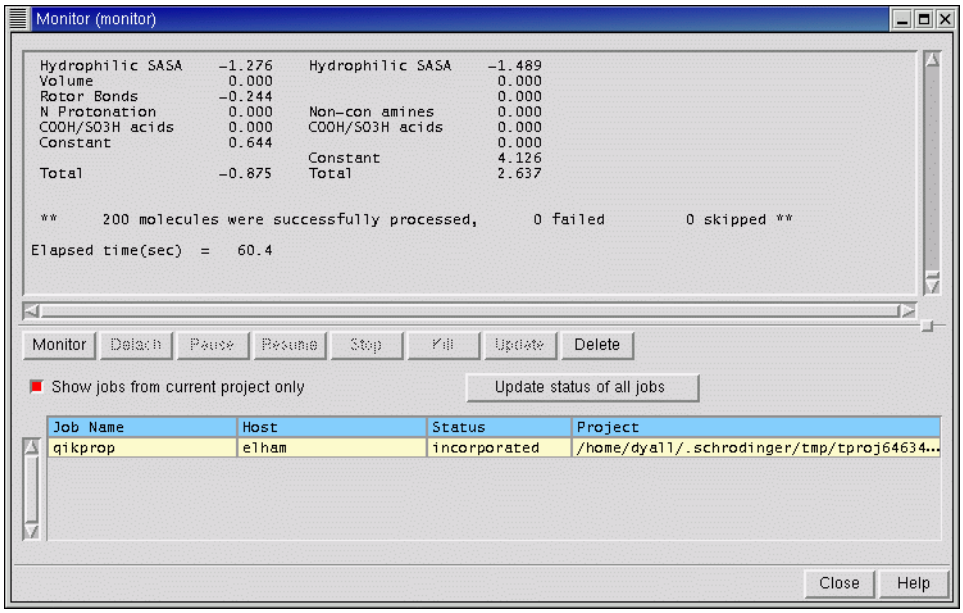


Figure 14.1. The Monitor ***panel.***

Table 14.2. Status descriptors in the Monitor *panel*

Status	Meaning
launched	The job was submitted and assigned a JobId.
submitted	The job is in a batch queue, waiting to be scheduled.
started	The environment for the job is being set up.
running	The job is running.
paused	The job has temporarily been suspended.
exited	The job has exited and is being cleaned up.
finished	The job finished successfully.
stopped	The job was stopped at an appropriate point at the user's request.
killed	The job was killed by someone (not necessarily the user).
died	The job failed during execution.
incorporated	The job results have been incorporated into a Maestro project.
fizzled	The job failed before it could be started.
stranded	Job control could not retrieve results or clean up the job.
unreachable	Job control could not connect to the machine running the job.

14.4 Managing Jobs

You can manage, or control, jobs from the Monitor panel or from the command line. The common tasks can be performed from the Monitor panel, but the full range of job control tasks is only available from the command line.

14.4.1 Controlling Jobs From the Monitor Panel

The Monitor panel allows jobs to be paused, resumed, or terminated using the Pause, Resume, Stop, and Kill buttons. Clicking Kill terminates the selected computational job immediately. The Stop button only affects MacroModel and Jaguar jobs, and is ignored by other jobs. When a job is stopped, the program saves results from the current stage of execution and cleans up before exiting. Pause and Resume can be used for all jobs.

14.4.2 Controlling Jobs From the Command Line

The job control utility allows you to perform a number of job control tasks from the command line. The syntax for job control utility commands is:

`$SCHRODINGER/jobcontrol` *command job_selection*

where *command* is the command for the operation you want to perform, and *job_selection* is the name of the specific job, if applicable. Valid commands are listed in Table 14.3:

The optional *job_selection* consists of one or more JobIds, job names, status codes or queries, or the keywords `all` or `active`. The default *job_selection* is all active jobs (jobs that are not finished), and is equivalent to using the keyword `active`. The keyword `all` means all jobs in your job database. The JobId is a unique identifier consisting of the name of the machine on

Table 14.3. Jobcontrol commands

Command	Action
`-abort`	emergency stop, abandon output files and the job record
`-cancel`	cancel a job that has been launched, but not started
`-delete`	remove a completed job from the database
`-dump`	show the complete job record
`-h[elp]`	describes the job control commands
`-int` *seconds*	interval for checking job status (default: 5 seconds)
`-kill`	terminate the job immediately
`-killnooutput`	terminate the job immediately and discard the output
`-list`	list the JobId, job name and status
`-monitor` *n*	ask for monitoring files to be sent every *n* seconds
`-pause`	suspend the job temporarily
`-ping`	verify that a running job responds to job control messages
`-recover`	try to retrieve results from a stranded job
`-refresh`	update the status of the job
`-resume`	continue running a paused job
`-show`	show more details of the job status
`-stop`	ask the job to stop itself as soon as possible (Jaguar, MacroModel only)
`-update`	ask for an update of the job results. (MacroModel only)
`-v[ersion]`	display program version and exit
`-view [-l` *log*`]`	view the job's log files in real time
`-wait`	wait for the job to finish before returning to the command prompt

which the job was launched, a sequence number, and a hexadecimal timestamp, e.g., `mirabelle-0-a1b2c3d4`. The job status codes and their meanings are listed in Table 14.2 on page 183.

The following examples illustrate different values of *job_selection*.

- To list all active jobs, showing their JobIds, job names, current status and the machine on which each is running, enter:

```
$SCHRODINGER/jobcontrol -list
```

- To list all the jobs in your job database that finished successfully, enter:

```
$SCHRODINGER/jobcontrol -list finished
```

- To list just the job whose JobId is `serv01-0-a1b2c3d4`, enter:

```
$SCHRODINGER/jobcontrol -list serv01-0-a1b2c3d4
```

- To list all jobs in your database with the job name `myjob`, enter:

```
$SCHRODINGER/jobcontrol -list myjob
```

- To list all jobs in your database, enter:

```
$SCHRODINGER/jobcontrol -list all
```

You can also use the wildcard character '?' to match a single unspecified character, or '*' to match zero or more unspecified characters. If you use either of these characters, you must protect them to ensure that they are interpreted by the `jobcontrol` script and not the UNIX shell. For example, you could enter either of the following commands to list all jobs whose job names start with `docklig`

```
$SCHRODINGER/jobcontrol -list docklig\*
$SCHRODINGER/jobcontrol -list 'docklig*'
```

More general queries are also possible. Formally, a query consists of one or more *conditions*, optionally separated by the Boolean operators AND, OR or NOT. If the operators are omitted, OR is assumed. A condition takes the form <field><op><value>, where <field> is one of the field names in the job record and <op> is one of the following:

=	equals
!=	is not equal to
=~	matches
!~	does not match

"Equals" means an exact match; "matches" means the string <value> is found.

The field names are listed in Table 14.4 on page 186. The fields that are most likely to be useful for queries are Name, Program, Host, Dir, JobHost, JobDir, Project, Status, and ExitStatus. The case of the field names is ignored, but the case of the <value> is significant. So, `Program=Jaguar` is the same as `program=Jaguar`, but `program=jaguar` would fail. Parentheses can be used to group conditions, but these must also be protected if used on the Unix command line. For example, to list all QSite jobs in your database that either died or were killed, enter the command

```
$SCHRODINGER/jobcontrol -list program=QSite AND < died OR
killed >
```

If a job is stranded, it might still be possible to re-establish contact with the job and incorporate the results. This can be done with the command:

`$SCHRODINGER/jobcontrol -recover` *jobid*

If this command fails, however, the job is cleaned up and the results are no longer available.

14.5 The Job Database

Information about each job is kept in the user's job database, which is stored in the directory `$HOME/.schrodinger/.jobdb`. The database contains a record for each job. You can determine what jobs are in the database by using the Maestro Monitor panel or the command-line job control utility.

14.5.1 The Job Record

Each job has a job record in the job database. The job record is a list of fields, one on each line, each consisting of a field name and its value. Many of these fields contain information that is only useful to the job control system, but a number may also be useful to users. Some of the latter are listed in Table 14.4

Table 14.4. Fields used in the job record

Field Name	Meaning
BackendPid	The PID for the program carrying out the calculation
Command	The command used to start up the actual calculation
Dir	The startup and output directory (on Host)
Envs	Environment variable settings for the job
Errors	Error messages from the job control system

Table 14.4. Fields used in the job record (Continued)

Field Name	Meaning
ExitStatus	The reason the calculation stopped
Host	The machine from which job was launched
InputFiles	Files copied from the output directory to the job directory at startup
JobDir	The directory in which the job is run
JobHost	The machine on which the job is run
JobId	The job's JobId
JobPid	The PID for the job's `jmonitor` process
JobUser	The user name under which the job is run
LaunchTime	The time at which the job was submitted
LogFiles	Monitoring files that grow throughout the job
MonitorFiles	Files copied from the job directory to the output directory during monitoring
MonitorInterval	The interval (sec.) between monitoring updates (0 if off)
Name	The job name
OutputFiles	Files copied from the job directory to the output directory at exit
ParentJobId	The JobId of the parent job, if this is a subjob
Processors	The number of processors used for a parallel or distributed job
Program	The program name
Project	The project name
StartTime	The time at which the calculation started running
Status	The current job status
StatusTime	The time at which Status was last updated
StopTime	The time at which the calculation stopped
StructureMonitorFile	The name of the monitoring file holding the molecular structure
StructureOutputFile	The name of the file holding the final molecular structure
User	The user name under which job was launched

To list the complete database record for a job, enter the command:

```
$SCHRODINGER/jobcontrol -dump jobid
```

14.5.2 Purging the Job Database

Normally, when running jobs from Maestro's project facility, the database record for a job is cleared once the job is incorporated into a Maestro project. Not all jobs can be incorporated, however; for this and other reasons job records might not get deleted automatically and the `.jobdb` directory can become quite large over time. The job control utility can be used to purge the job database of records for completed jobs. For example, the following command purges the entire database:

```
$SCHRODINGER/jobcontrol -delete all
```

This command only affects completed jobs: running jobs cannot be deleted. However, you should be careful not to delete completed jobs whose output you still intend to incorporate into a Maestro project.

The job database is automatically checked for jobs that have finished whenever you start a new job. If the job is older than a threshold time, it is deleted from the database. You can set this threshold time in the environment variable `SCHRODINGER_JOBDB_CLEANUP`. The minimum time is 1 second, and the default time is 1 week. The default unit is seconds, but you can specify a time in minutes, hours, or days by appending m, h, or d to the value, for example, 7d, 168h, or 5m.

14.6 Running Jobs From the Command Line

For most purposes, you can start jobs from Maestro. If you want to run jobs from the command line or from a script, the job control facility recognizes a number of command line options that can be used to control the behavior of the job. These options are summarized in Table 14.5. Some of the options are described in more detail below.

Table 14.5. Command options

Option	Description
`-DISP` *policy*	Set the project incorporation policy for this job: `ignore`, `append`, or `replace`. Requires `-PROJ`.
`-HOST` *hostname*	Run a job on the specified host or submit a job to the specified batch queue. Default: run on the local host.
`-LOCAL`	Write temporary files to the job startup directory instead of the scratch directory. Default: write temporary files to the scratch directory.
`-PROJ` *name*	Assign the job to a Maestro project.
`-TMPDIR` *directory*	Specify the scratch directory for the job.

Table 14.5. Command options (Continued)

Option	Description
`-USER` *username*	Specify the user name to be used for remote jobs. Must be used with `-HOST`. Default: use the same user name as on the submission host.
`-WAIT`	Wait for the job to finish before returning to the command prompt (replaces `-w`). Default: return to the command prompt immediately.

You can also obtain information for each program about the hosts you can use, and which version of the program will be run. These options are listed in Table 14.6 .

Table 14.6. Information options.

Option	Description
`-DEBUG` `-DDEBUG`	Show the details of operation of the toplevel script. Show the verbose details of operation of the toplevel script.
`-ENTRY`	Show the section of the `schrodinger.hosts` file that will be used for this job.
`-HOSTS`	List the hosts that are available for calculations.
`-LIST` [*version-options*]	List the available versions of the program that can be run on the host specified by `-HOST`. If no host is specified, the local host is used. If v*ersion-options* is `-ALL`, list all available versions, even if not compatible with the specified host.
`-WHICH` [*version-options*]	Show which version of the program and of the `mmshare` library would be used for the given version options.
`-WHY` [*version-options*]	Gives information about why the specified version was selected.

The allowed values of *version-options* for the information options are listed in Table 14.7.

Table 14.7. Version options

Option	Description
`-ARCH` *platform*	Platform code, e.g., `Linux-x86`, `IRIX-mips4`.
`-COMPAT` *executable*	Select the version that is compatible with the specified executable, for which the full path must be given.
`-REL` *version*	Release version number: `v42`, `v4.2`, `42`, `v42062`, `41059`, `v4.1.049` are all acceptable forms.
`-VER` *pattern*	Pattern to match in the path to the executable.

The -WAIT option

All jobs are run in the background automatically, dissociated from the terminal session (or application) from which they were launched. As a result, the job continues to run even if you quit Maestro or the terminal session from which you launched the job. For command-line jobs, this means that the UNIX command prompt is returned immediately, without waiting for the job to finish. This behavior is not always desirable, especially if you want to run the job in a script, in which some subsequent action can be taken only after the job finishes. The command-line option -WAIT can be used to prevent the command prompt from returning until after the job finishes. For example:

```
$SCHRODINGER/bmin -WAIT job_name
```

Even with this option, however, the calculation is still placed in the background, so pressing CTRL+C or CTRL+Z does not affect it. If you submit a job to a batch queue, however, the command prompt is returned immediately, regardless of the presence of the -WAIT option, because this option applies to the running of the program, not the submission of the job to the batch queue.

The -HOST Option

Jobs can be submitted to a remote host using the -HOST option to specify the remote host name. For example:

```
$SCHRODINGER/bmin -HOST hostname jobname
```

For programs that can run a single job in parallel or distribute several jobs over a number of processors, the -HOST option can be used to specify the list of hosts to be used. The host list is a list of host entry names, separated by spaces. The list must be enclosed in quotes if there is more than one host specified.

Each host entry name may also specify a processor count, using the syntax:

hostname:*processors*

An example of a host list specification is:

```
-HOST "florence:2 glinda"
```

The first host in the list is always the main host for the job, that is, the host on which the main process for the parallel or distributed job executes.

The -LOCAL Option

For some applications, like MacroModel, you can request temporary files to be written to the job's startup directory, instead of in the scratch directory with the -LOCAL option. For example,

```
$SCHRODINGER/bmin -LOCAL job_name
```

Not every application supports this option. When it is supported, it may be used for both local and remote jobs. If you run a remote job with the `-LOCAL` option, it is important to make sure that the startup directory is accessible on the remote machine.

14.7 Incorporation of Job Output

When project entries are used as input for jobs, the structure and property output can be incorporated into the project. You can specify how you want the results to be incorporated in the Start dialog box (see Section 14.2 on page 181). To open the Start dialog box, click the Start button in the panel used to set up the job. The three incorporation options and their effects are described below.

- Append new entries—New entries are added to the end of the Project Table. The names for the new entries have `-inc`*n* appended, where *n* is a number used to ensure uniqueness of the name.
- Replace existing entries—Incoming entries replace pre-existing entries of the same name.
- Do not incorporate—Output files are written to the working directory but structure and property data are not incorporated into the Project Table. You can import the results later using the Import panel. See Chapter 2 for more information on importing structures.

Incorporation of job output into the project takes place only from monitoring mode. If you are monitoring a job launched from the current project, and that job finishes during the monitoring session, incorporation is immediate. If you are not in monitoring mode when the job finishes, you must select and then monitor the job before the results are incorporated.

When a job is incorporated, the first structure in the job output is displayed in the Workspace. Incorporated entries are in a contiguous block, and the entry list is scrolled to the first of these entries.

Incorporation can be undone. Undoing incorporation removes the new entries from the project and restores the Workspace to the state it was in just before monitoring mode was entered.

Computational programs normally propagate entry names (as well as other properties) from their input into their output structures. Where the relationship is one-to-many, as in a conformational search, consecutive structures in the output file have identical entry names. If the job is run with the “append” incorporation mode, the names are identical to that of the input entry.

Because project entries must have unique names, the project facility uses automatic rules for creating unique entry names when the output entries are incorporated. When an entry is incorporated, the suffix `-inc`*n* is added to the entry name. The value of *n* starts at 1 and is incre-

mented for each incorporation event. For instance, if the input entry was `ligand1` and the job output contained a single entry, also named `ligand1`, the output entry would be given the name `ligand1-inc1`.

Multiple consecutive entries bearing the same entry name incorporated from a single file are distinguished using a "dot suffix." Thus, if the output of the above job contained multiple consecutive entries, all named `ligand1`, then, on import, they would be renamed `ligand1-imp1.1`, `ligand1-imp1.2`, etc.

See Appendix C for information on the suffixes used in entry naming.

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 Balloon help. Manuals in PDF format are included with the product distribution, and each product has an FAQ page on the Schrödinger web site.

15.1 Maestro Online Help

If you have any difficulty performing a particular operation within the Maestro interface, look for answers first in the online help, which is presented in the Help panel.

The Help panel contains two folders for locating help topics, the Search folder and the Categories folder. Below these folders, the topic name appears in the Topic text box, and the help topic is displayed in the text area below the topic title.

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.

For general information, open the Help panel and start a search. To open the Help panel, choose Help from the Help menu, or press CTRL+H in the Workspace.

For help on a particular panel's features, click the Help button in the lower right corner of the panel. The Help panel opens with the relevant topic displayed.

15.1.1 Locating a Topic by Searching

The Search folder allows you to search for a topic using a search string. Type the string in the Search For text box and press the RETURN key or click the Search button. If there are any topics in the help file that contain the search string you entered, they are listed in the Topics which match search list. The search results are sorted in alphabetical order. By default, the last entry in the list is highlighted. This does not mean that the highlighted topic most closely matches the query word. To view a topic, double-click on its name in the list, or click on the name once and then press the RETURN key.

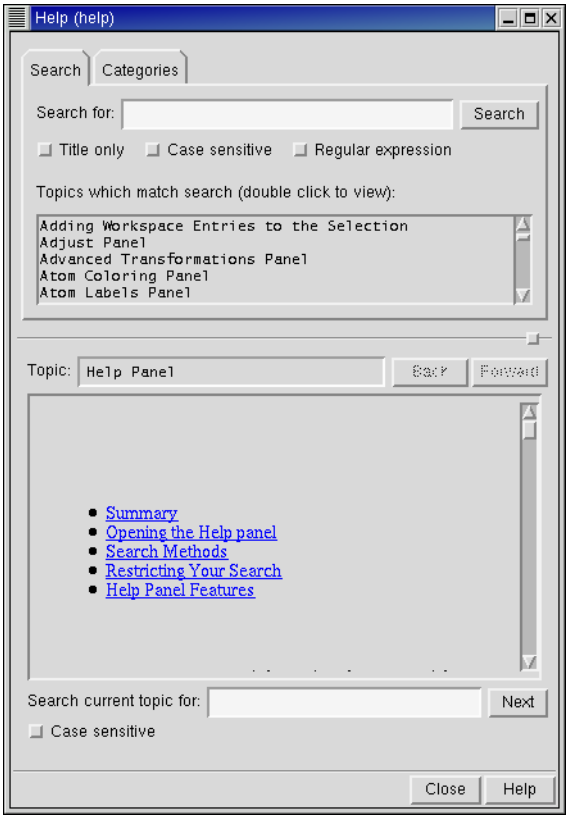


Figure 15.1. The Help ***panel showing the*** Search ***folder.***

You can restrict or enhance your search by selecting the following options:

- Title Only: The search is restricted to the topic titles.
- Case Sensitive: The case is matched exactly in the search.
- Regular Expression: Allows the use of UNIX regular expressions in the search.

15.1.2 Locating a Topic by Category

Searching for help by category is helpful when you do not know which keywords may produce the desired topic. Select the option from the Help Categories: menu that corresponds to the group of topics you would like to browse. A list of relevant topics is displayed in the Topics in this category list. The topics in the list are arranged in alphabetical order and the last entry in the list is highlighted. To select a topic, double-click its name, or click its name and press ENTER.

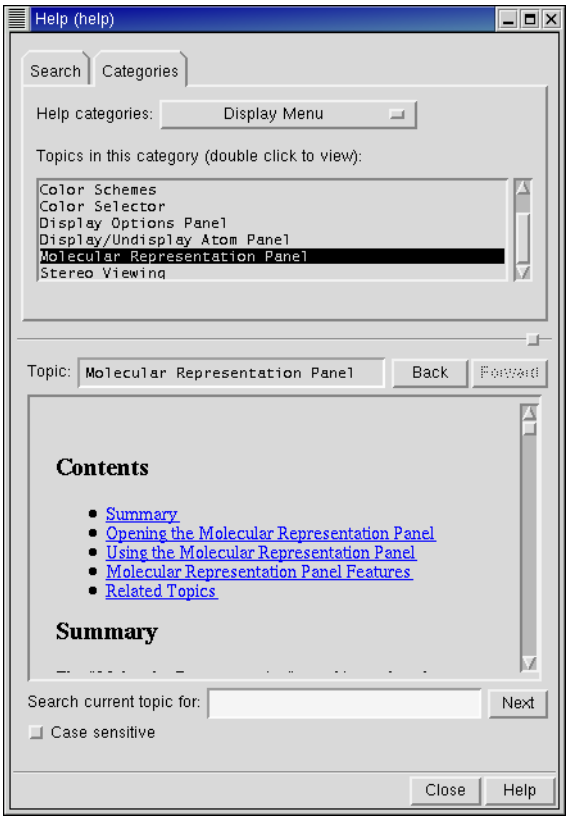


Figure 15.2. The Categories ***folder of the*** Help ***panel.***

15.1.3 Searching Within a Topic

If you want to locate a string in the topic text, type the string in the Search current topic for text box and press ENTER. To locate the next occurrence of the string, press ENTER again or click Next. You can match the exact case of the search string by selecting Case sensitive.

15.2 Context-Sensitive Help

In addition to the Help facility, Maestro has some other supporting help features. They are described below.

Auto-Help

The Auto-Help window is located just below the title bar of the main window. The Auto-Help facility provides automatic context-sensitive help. For example, when you open the Atom

Labels panel from the Display menu, Auto-Help prompts you to pick an atom to label. Auto-Help is not available for all operations.

Balloon Help

Balloon Help consists of a floating text box containing context-sensitive help that appears when the cursor is allowed to rest on an object. The balloon disappears when you move the mouse. You can temporarily disable Balloon Help using the Show Balloon Help item on the Help menu. Balloon Help is not available for all interface components.

15.3 Manuals

If you have difficulty installing Maestro, see the *Schrödinger Product Installation Guide*. If you have questions about a computational program that you have purchased, see the *User Manual* or *Reference Manual* for that program. Manuals are available in PDF format on the program CD and the Schrödinger web site.

15.4 The Schrödinger Web Site

The Schrödinger web site, http://www.schrodinger.com, contains information about all our products. In the Support pages, you can find the manuals in PDF format (http://www.schrodinger.com/Support/pdf.html) and a list of frequently asked questions (http://www.schrodinger.com/Support/faqs.html) for each of the products. The manuals on the web site are the most up-to-date. The manuals page contains links to corrections and additions to the documentation. The web site also contains information about product releases and software updates. Consult the web site for the most recent information on a product.

15.5 Technical Support

If you have questions that have not been answered from any of the above sources, contact Schrödinger using the information below. Generally, e-mail correspondence is best because you can send relevant machine output.

Schrödinger
E-mail:help@schrodinger.com
USPS:1500 SW First Ave. Suite 1180, Portland, OR 97201
Phone:(503) 299-1150
Fax: (503) 299-4532
WWW:http://www.schrodinger.com
FTP: ftp://ftp.schrodinger.com

When sending e-mail messages, please include the following:

- All relevant user input and machine output
- Software purchaser (company, research institution, or individual)
- Primary software user
- Computer platform type
- Operating system with version number
- Software version number
- Maestro version number
- mmshare version number

Much of the machine and system information listed above can be produced by entering the following command at a shell prompt:

```
$SCHRODINGER/machid
```

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 section will give 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 proceeded 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 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.*
`s_m_grow_name`	*The name used by the Maestro structure builder.*

`i_m_atomic_number`	*The atomic number.*
`i_m_formal_charg`	*The formal charge.*
`i_m_representation`	*The representation used to draw this atom.*
`i_m_visibility`	*A flag to indicate whether this atom is displayed in Maestro or not.*
`s_m_atom_name`	*The user-specified atom name.*
`:::`	*The separator for the end of the data items.*

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.*

`m_bond[36] {`	*The bond block. There are 36 bonds.*
`i_m_from`	*The atom the bond is from.*
`i_m_to`	*The atom the bond is to.*
`i_m_order`	*The bond order.*
`i_m_from_rep`	*The graphical representation for the "from" half-bond.*

```
    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`. We continue to use the original MacroModel atom types for most applications, but now have a mechanism for easily adding new types. The list of explicitly supported atom types has been expanded to include:

Li^{+}, Na^{+}, K^{+}, Rb^{+}, Cs^{+}, Ca^{2+}, Ba^{2+}, Mg^{2+}, Mn^{2+}, Mn^{3+}, Mn^{4+}, Mn^{5+}, Mn^{6+}, Mn^{7+}, Fe^{2+}, Fe^{3+}, Co^{2+}, Co^{3+}, Ni^{2+}, Ni^{3+}, Cu^{+}, Cu^{2+}, Zn^{2+}, Mo^{3+}, Mo^{4+}, Mo^{5+}, Mo^{6+}, and Cl^{-}.

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-v`*version*`/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. See the *MacroModel Reference Manual* for a description of the `atom.typ` file and how to add atom types.

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 heteroatoms.

Table B.1. Atom types and equivalents

			Equivalencies		
No.	**Symbol**	**Description**	**MM2/ MM3**	**Charmm**	**Amber**
1	C1	Carbon - sp			
2	C2	Carbon - sp^2	2,3	CT,C	C, C*, CA, CB, CC, CM, CF, CG, CN
3	C3	Carbon - sp^3	1	CT	CT
4	CA	United atom CH - sp^3		CH1E	CH
5	CB	United atom CH_2 - sp^3		CH2E	C2
6	CC	United atom CH_3 - sp^3		CH3E	C3
7	CD	United atom CH - sp^2		CR1E	CD, CE, CJ, CP
8	CE	United atom CH_2 - sp^2			
9	CF	United atom CH - sp			
10	CM	Carbanion (C^-)			
11	CP	Carbocation (C^+)	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^- (alkoxide, carboxylate)	47		OC
19	OW	United atom H_2O		OH2E	
20	OP	Oxonium (sp^2) =[O^+]–			
21	OQ	Oxonium (sp^3) R_3O^+			
...					
23	O0	Any oxygen			
24	N1	Nitrogen - sp	10		

Table B.1. Atom types and equivalents (Continued)

			Equivalencies		
No.	**Symbol**	**Description**	**MM2/ MM3**	**Charmm**	**Amber**
25	N2	Nitrogen - sp^2	9	N, NR, NP, NH1, NH2	N, NB, NC, N*, N2
26	N3	Nitrogen - sp^3	8	NH3	NT
27	NA	United atom NH - sp^3			
28	NB	United atom NH_2 - sp^3		NH1E	
29	NC	United atom NH - sp^2			
30	ND	United atom NH_2 - sp^2		NH2E	
31	N4	N^+ - sp^2		NC2	NA
32	N5	N^+ - sp^3	39		N3
33	NE	United atom NH^+ - sp^3			
34	NF	United atom NH_2^+ - sp^3			
35	NG	United atom NH_3^+ - sp^3		NH3E	
36	NH	United atom NH^+ - sp^2			
37	NI	United atom NH_2^+ - sp^2		NC2E	
38	NM	N^- - sp^3			
39	NP	N^- - sp^2			
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-Cation	48 MM3 (none in MM2)		H3
45	H5	H-Anion			
...					
48	H0	Any hydrogen			
49	S1	Sulfur	15,17,18	S	S, SH
50	SA	United atom SH		SH1E	

Table B.1. Atom types and equivalents (Continued)

			Equivalencies		
No.	**Symbol**	**Description**	**MM2/ MM3**	**Charmm**	**Amber**
51	SM	S^- (thiolate anion)			
52	S0	Any Sulfur		S	
53	P0	Phosphorus	25		P
54	B2	Boron - sp^2	26		
55	B3	Boron - sp^3	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^+			Li
66	Na	Na^+		SOD	Na
67	K0	K^+		POT	K0
68	Rb	Rb^+			Rb
69	Cs	Cs^+		CES	
70	Ca	Ca^{+2}		CAL	
71	Ba	Ba^{+2}			
72	Mg	Mg^{+2}		MG	
73	M2	Mn^{+2}			
74	M3	Mn^{+3}			
75	M4	Mn^{+4}			
76	M5	Mn^{+5}			
77	M6	Mn^{+6}			

Table B.1. Atom types and equivalents (Continued)

			Equivalencies		
No.	**Symbol**	**Description**	**MM2/ MM3**	**Charmm**	**Amber**
78	M7	Mn^{+7}			
79	f2	Fe^{+2}			
80	f3	Fe^{+3}			
81	o2	Co^{+2}			
82	o3	Co^{+3}			
83	n2	Ni^{+2}			
84	n3	Ni^{+3}			
85	c1	Cu^{+}			
86	c2	Cu^{+2}			
87	Zn	Zn^{+2}			
88	m3	Mo^{+3}			
89	m4	Mo^{+4}			
90	m5	Mo^{+5}			
91	m6	Mo^{+6}			
...					
100	SP	S^{+}			
101	S2	Sulfur - sp^2			
102	Cm	Cl^{-}		CLA	
...					
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

Entry Suffixes

The entry names within a project must be unique. Maestro uses various suffixes to ensure that the names are unique. Numbers are added after the suffix to make the name unique. Maestro adds a suffix when certain operations are performed on entries. These suffixes are listed in Table C.1.

Table C.1. Entry name suffixes

Operation	Suffix	When Added
merge projects	`-mrg`	name conflict
import	`-imp`	always
job incorporation	`-inc`	always
create from Workspace	`-wse`	name conflict
rename entry	`-re`	name conflict, or multiple entries selected
combine entries	`-com`	name conflict
disassociate	`-dis`	always
duplicate	`-dup`	always

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 utility programs are installed in `$SCHRODINGER/utilities`. UNIX conventions are used for the command syntax—see the Document Conventions on page xiii for more information.

D.1 Structure Conversion

This section describes the utilities available for conversion between various file formats for molecular structures. These utilities are used by Maestro for structure conversion when importing or exporting structures.

D.1.1 Conversions to and From MacroModel Format

`maemmod`

Convert files from Maestro format (`.mae`) to MacroModel format (`.dat`).

Syntax:

`maemmod` *maestro-file* *mmod-file*

`mmodmae`

Convert files from MacroModel format to Maestro format.

Syntax:

`mmodmae` *mmod-file* *maestro-file*

`mmio_convert`

Compress and uncompress MacroModel format files.

Syntax:

`mmio_convert` [*infile* [*outfile*]]

D.1.2 Conversions to and From Mol2 Format

mmodmol

Convert files from MacroModel format to Sybyl Mol2 format.

Syntax:

`mmodmol [`*input-file*`] [`*output-file*`]`

If the input file is not specified, input is taken from standard input. Likewise, if the output file is not specified, output is sent to standard output.

Example:

`mmodmol` *myfile*`.dat > `*myfile*`.mol2`

molmmod

Convert files from Sybyl Mol2 format to MacroModel format.

Syntax:

`molmmod [`*input-file*`] [`*output-file*`]`

If the input file is not specified, input is taken from standard input. Likewise, if the output file is not specified, output is sent to standard output.

Example:

`cat` *myfile*`.mol2 | molmmod >` *myfile*`.dat`

D.1.3 Conversions to and From PDB Format: pdbconvert

This section describes the command-line utility version of the program that converts files between PDB, MacroModel, and Maestro formats. For information on PDB conversion within the Maestro GUI, see Section 2.1.3 on page 21.

Syntax:

```
pdbconvert [options] {-ipdb|-imm|-imae} inputfile
      {-opdb|-omm|-omae} outputfile
```

`-ipdb` *inputfile*	Input file in PDB format
`-imm` *inputfile*	Input file in MacroModel format
`-imae` *inputfile*	Input file in Maestro format

`-opdb` *outputfile*	Output file in PDB format
`-omm` *outputfile*	Output file in MacroModel format
`-omae` *outputfile*	Output file in Maestro format

Options:

`-data` *datafile*	Read *datafile* for more default data
`-model` *number*	Specify an input structure other than the first
`-no_color`	Color atoms by type, not "error code"
`-no_dup_conect`	Don't take duplicate CONECT records to mean multiple bonds
`-no_renum`	Retain atom indices from the MacroModel file
`-warn_h`	Include hydrogens in missing atom and unrecognized atom name warnings

Conversion Behavior for Importing PDB

Where multiple atomic coordinates exist for a single PDB entry, Maestro chooses the atoms with the highest occupancy ratio.

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 Section 2.1.3 on page 21.

Note: Unlike Maestro and SD files, PDB files do not support multiple structures, only multiple sets of coordinates for the same molecule, e.g. different NMR refinements. Certain PDB structures do not follow the PDB standard and have varying number of atoms in different MODELs. Do not import these PDB structures, as they will cause Maestro to fail.

Conversion Error Codes for `pdbconvert`

When running `pdbconvert` from UNIX, you will receive numerical messages (2, 1, 0) indicating the status of an attempted PDB conversion. These messages are equivalent to Maestro's dialog box warnings. The message numbers are defined as follows:

2 (ERROR): A fatal error occurred, and no Maestro file was generated. Check disk permissions and disk space.

1 (WARNING): A Maestro file was created, but an error at or above the base error level was returned. At the default base error level, this value is returned when red or blue atoms are present, and for orange atoms if the duplicate CONECT record convention is not followed. See Table 2.2 on page 22 for a description of the atom colors.

0 (OK): A Maestro file was generated without any errors at or above the base error level.

Using Templates for Non-Standard Residues

The `pdbconvert` program has been supplied with connectivity and bond order information for standard residues. For non-standard residues, the program predicts connectivity, but not bond order. However, if the connectivity and bond order information for a non-standard residue is known, it can be used to read in the PDB file. Create a new file that contains a template with this information (see example below).

```
TEMPLATE{
"ALA "
" N " " CA " 1
" N " " H " 1
" CA " " CB " 1
" CA " " C " 1
" C " " O " 2
" HA " " CA " 1
"1HB " " CB " 1
"2HB " " CB " 1
"3HB " " CB " 1
}
```

A connectivity template must begin with `TEMPLATE{` and end with a closing brace `}`. Each line in the template should specify two atom names, followed by a bond order. Templates for ligand molecules can also be created. To specify a template file to be used by `pdbconvert`, use the `-data` option.

The standard residue template file for `pdbconvert` can be viewed at

`$SCHRODINGER/mmshare-v`*version*`/data/mmpdb.ini`.

D.1.4 Conversions to and From SD Format: sdconvert

Convert between MDL SD, Maestro, and MacroModel format files.

Syntax:

```
sdconvert [options] {-isd|-imm|-imae} inputfile
        {-osd|-omm|-omae} outputfile
```

`-isd`	Input file in SDfile format
`-imm`	Input file in MacroModel format
`-imae`	Input file in Maestro format
`-osd`	Output file in SDfile format
`-omm`	Output file in MacroModel format
`-omae`	Output file in Maestro format

Options:

`-a`	Append structures to the output file
`-all`	Convert all structures (synonym for `-n 1:)`. This is the default action.
`-h`	Show usage summary
`-n` *structs*	Specify a comma delimited series of colon-separated ranges and single values to convert. For example:

`1:10,14`	(structures 1 through 10 and 14)
`2:`	(structure 2 through end of file)
`:5,13:18`	(structure 1 through 5, and 13 through 18)

For multiple `-n` options, the right-most takes precedence.

Example:

```
$SCHRODINGER/utilities/sdconvert -n 1: -isd lig.sdf -omae
   lig.mae
```

D.2 Structure Extraction

This section describes utilities for extracting a subset of structures from a structure file. The first two utilities, `maesubset` and `sdsubset`, extract structures by index. The third utility, `propfilter`, extracts structures from a Maestro-formatted file based on values of properties.

`maesubset`

Extract a subset of structures from a Maestro format input file.

Syntax:

```
maesubset -n range full.mae > subset.mae
maesubset [-h] [-v]
```

range	`1:200`	(structures 1 through 200)
	`50:`	(structures 50 through end of file)
	`"1:5, 14"`	(structures 1 through 5 and 14)

Options:

`-h`	Show usage summary
`-v`	Show the version number of this utility.

sdsubset

Extract a subset of structures from an SD format input file.

Syntax:

```
sdsubset -n range full.sdf > subset.sdf
sdsubset [-h] [-v]
```

range	`1:200`	(structures 1 through 200)
	`50:`	(structures 50 through end of file)
	`"1:5, 14"`	(structures 1 through 5 and 14)

Options:

`-h`	Show usage summary.
`-v`	Show the version number of this utility.

propfilter

Filter Maestro-formatted input file based on properties. Can filter on QikProp property names or internal Maestro property names.

Syntax:

```
propfilter [options] input-file
propfilter [-h] [-n] [-v]
```

Options:

`-e` *filter_condition*	A single filter condition. Multiple such conditions may be specified.
`-f` *filter_file*	Input file listing filter conditions to be used.
`-h`	Show usage summary.
`-n`	List the recognized property names. (The input file is not processed.)
`-o` *output_file*	Filename for output Maestro- formatted file. If no output file is specified, structures are written to the file `propfilter.mae`.
`-v`	Show the version number of this utility.

Filter conditions must be specified in the form "*name op value*", or just *name*. Here, *name* is the name of a property or descriptor.

name

- For QikProp properties, the standard CSV-file header name may be used, e.g., `MW` or `#nstars` or `dip^2/V`
- The internal Maestro property names may also be used, e.g., `r_qp_mol_wt`, or `i_qp_n_stars` or `r_rp_d2ov`.

op

The conditional operator *op* must be one of the following:

```
>    >=   <    <=
==   !=   ~    !~
```

and it must be surrounded by white space. The ~ and !~ operators perform pattern matching using regular expressions.

If a condition is simply *name*, then the named property is required to exist, but it may have any value.

If filter conditions are supplied in an input filter file, there must be one condition per line. Lines that start with # are treated as comments. Blank lines are ignored.

D.3 Display of Properties

proplister

List properties in Maestro-formatted files.

Syntax:

`proplister [`*options*`] `*input-files*

Options:

`-a`	Report *all* the properties found in the input files.
`-c`	Write properties to a CSV file.
`-h`	Show usage summary.
`-l`	List the names of all the properties found in the input files.
`-n`	List the property names for which user-friendly names are known. (Input files are ignored).
`-p` *property_names*	Names of properties to report. If more than one property is given, the names must be quoted. e.g., `-p "title MW"`. This is the same as `-p title -p MW`.
`-v`	Show the version number of this utility.

D.4 Structure Preparation

applyhtreat

Apply a hydrogen treatment (add or delete hydrogens) to one or more structures in a Maestro format file.

Syntax:

`applyhtreat` *input-file* *output-file* `["`*treatment-name*`"] ["`*ASL-expression*`"]`

Options:

Allowed treatment names:

```
All-atom with Osp3/Nsp3-Lp
All-atom with No-Lp
Csp3 United-atom with S-Lp
Csp3 United-atom with No-Lp
```

```
All-atom with S-Lp
C sp2/sp3 United-atom with No-Lp
C sp2/sp3, N,O,S United-atom with No-Lp
```

Default treatment: `All-atom with No-Lp`

The treatment name must be enclosed in quotes. The ASL expression can be used to specify a range of atoms to which the treatment is to be applied. It must also be enclosed in quotes.

The `applyhtreat` utility can be used to delete or add hydrogens to one or more structures in a Maestro format file, consistent with the hydrogen treatment option that you provide. A *hydrogen treatment* is a protocol that determines which atoms are to have hydrogens and/or lone pairs attached. Several different treatments are supplied. Each of these treatments is associated with a particular molecular mechanics force field. However, some treatments are suitable for several force fields. SeeTable 3.1 on page 46 for information on the correspondence of treatments to force fields.

The `applyhtreat` utility is used by Maestro when a hydrogen treatment is applied in the Hydrogen Treatment folder of the Build panel. See Section 3.8 on page 46 for more information.

Note:

- Hydrogen addition or deletion takes place only as necessary to make the structure consistent with the selected hydrogen treatment. For example, if the specified treatment option calls for all atoms to have hydrogens and the structures in the input file already have hydrogens on all atoms, no changes will be performed.
- Maestro changes the default hydrogen treatment automatically if the force field is changed. The new hydrogen treatment will be one of those acceptable for the newly selected force field.

D.5 Unique Names

`unique_names`

This program takes files in Maestro format and adjusts the numeric suffixes for structure titles and entry names to make them unique. This is useful for post-processing output from programs, such as LigPrep and MacroModel, that produce structures with identical titles and entry names.

Note: If the structures in the input file already have unique names, these names might not be preserved if they only differ from a non-unique name by the numeric suffix.

Syntax:

`unique_names` *input-file* *output-file*

Example:

The file `ligprep.mae` contains the following structures:

Entry Name	Title
entry	title
entry	title2
entry	title2
entry	title3

To create unique titles and entry names for these four structures, enter the following command:

```
unique_names ligprep.mae ligprep-out.mae
```

The structures in the resulting file `ligrpep-out.mae` now have unique names:

Entry Name	Title
entry	title
entry1	title2
entry2	title3
entry3	title4

Color Ramps

With Maestro, you can map any volume data onto any surface. In addition to the default color ramps provided with Maestro, you can also create your own color ramps.

To create a color ramp named Red_Orange_Yellow_Green_Blue :

1. Copy the ramp definition files to your local resource directory:

   ```
   cp $SCHRODINGER/maestro-vversion/data/res/ramp.res \
       $HOME/.schrodinger/maestroversion/
   cp -r $SCHRODINGER/maestro-vversion/data/res/ramps \
       $HOME/.schrodinger/maestroversion/
   ```

2. Edit the `$HOME/.schrodinger/maestroversion/ramp.res` file to define the new color ramp by adding the following lines to the end of the file:

   ```
   # Rainbow Color ramp
   rainbow
   Red_Orange_Yellow_Green_Blue
   rainbow.rmp
   ```

3. In the `$HOME/.schrodinger/maestroversion/ramps` directory, create a new ramp file called `rainbow.rmp` that contains the following lines:

   ```
   # Number of colors
   # 5
   # Color names for all colors of this color ramp
   red
   orange
   yellow
   green
   blue
   ```

4. Restart Maestro.

5. Choose Surface Table from the Surfaces submenu of the Display menu in the main window and click the Display Options button.

   The Red_Orange_Yellow_Green_Blue ramp should now be available in the Color ramp option menu at the bottom of the panel.

Note: You can use any color in the Maestro color palette. To see what is available, choose Atom Coloring from the Display menu and select the Atom Color folder. You can view the colors by palette or by name.

A single color may appear more than once. So you could extend the range for the endpoints by defining the following color ramp:

```
# Number of colors
# 7
# Color names for all colors of this color ramp
red
red
orange
yellow
green
blue
blue
```

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F.1 NCSA HDF5 Software Library and Utilities

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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.

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.

ESD—Entry Selection dialog box.

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.

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.

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.

synchronization—updating the project with changes made in the Workspace. The default is to perform synchronizations automatically.

volume—a set of data points on a three-dimensional grid for a property that is a function of the three spatial coordinates.

Workspace—The open area in the center of the Maestro main window in which structures are displayed.

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