

The KING manual

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Abstract

KING (Kinemage, Next Generation) is an interactive system for three-dimensional vector graphics. It supports a set of graphics primitives that make it suitable for many types of graphs, plots, and other illustrations; although its first use was to display macromolecular structures for biophysical research. KING builds on MAGE, JAVA-MAGE, and the “kinemage” (kinetic image) concept to deliver a full-featured Java application with a user-friendly interface and integrated editing features. It also operates as a Java applet to promote easy access to kinemages from a web browser.

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Chapter 1

Getting started

1.1 What is a kinemage?

A kinemage is a “kinetic image,” an interactive, three-dimensional illustration. Because kinemages contain simple geometric objects — points, lines, spheres, *etc.* — they are suited to a great variety of subjects, from simple sketches to sophisticated plots to detailed schematics of 3-D objects. Their strength is in *selective* presentation of information — they were originally intended as an alternative to flat, static illustrations in scientific journals.

In fact, kinemages were first created as a way of visualizing macromolecular structures, particularly x-ray crystal structures of proteins. However, such a kinemage is a *drawing* of a molecule, albeit a 3-D drawing, and not the molecule itself. Thus, the kinemage lacks most of the information in a PDB file, and kinemage display program cannot read PDB files directly. Since their creation, kinemages have been extended to a variety of other fields, from the social sciences to ecology to education.

The kinemage concept is the brainchild of Drs. David and Jane Richardson at Duke University in Durham, North Carolina, USA. Their website is at <http://kinemage.biochem.duke.edu>.

1.2 Starting the KiNG program

If you’re reading this, you may already have KiNG running. In that case, feel free to skip this section. If not, we’ll guide you through getting KiNG up and running on your system.

1.2.1 Download KiNG

If you don’t already have a copy of KiNG, you can download it from <http://kinemage.biochem.duke.edu>. Even if you have a copy already, you might check periodically for new version that add features and fix bugs. If you run on a Windows or Linux machine

and aren't already knowledgeable about Java technology, we recommend downloading the package that includes a Java Virtual Machine in the bundle. (This isn't an issue for Macintosh owners.)

If you just want to run KiNG as an applet on MolProbity or some other web page, you can skip this step. You can always download a copy later if you want to run it off-line.

1.2.2 Make sure you have Java

KiNG is written in the Java programming language, and so requires that the Java libraries (version 1.3 or later) be present on your computer in order for it to run. Newer Apple computers (those running Mac OS X) come with Java. Most PCs do not, though recently several manufacturers have agreed to pre-install Java on their new computers. Look for the coffee-cup icon in your Windows task bar or in the Control Panel.

If you don't have Java, you may have downloaded a copy of KiNG that was bundled with its own installation of Java. If you ran the InstallAnywhere installation program, this is the copy you have; don't worry about downloading and installing another copy of Java.

If you don't have Java and you didn't download the bundled version of KiNG, point your web browser to <http://java.sun.com/getjava/index.html>. The software is free and available for Windows, Linux, and Solaris computers. We recommend getting the newest version that is available (1.4.2 as of this writing).

1.2.3 Launch KiNG

Launching KiNG is as simple as double clicking on the "KiNG" icon. If you didn't download a package with an installer, *etc.* you may need to click on `king.jar` instead.

For Unix types who want a shell script, we recommend something like this:

```
#!/bin/sh
exec java -Xms32m -Xmx128m -jar /home/ian/bin/jars/king.jar "$@"
```

The `-Xms` and `-Xmx` switches control the amount of memory initially allocated to the Java program and the maximum memory it can consume. The default maximum of 64 MB should be enough for almost any kinemage, but a few of the largest require more (hence the `-Xmx128m` recommendation).

If you just want to run KiNG as an applet from a web page, you can just visit that web page now. If you don't see the "Kinglet" logo after a minute or two, make sure your browser is properly configured to work with Java. How you do this depends on which browser you have; consult its documentation for details.

1.3 Opening a kinemage

If you already have a kinemage you want to look at, this step is simple: just choose Open from the File menu, and select the kinemage you'd like to view. If you don't have anything to look at right now, don't worry! Choose Help | Built-in kinemages,

and select one of the provided files to explore. See 8 on page 32 for more places to get kinemages from.

1.4 Basic kinemage reading: Using KiNG to view a kinemage

1.4.1 Basic interaction

1.4.1.1 Moving the kinemage around

A kinemage is a dynamic, 3-D illustration. The best way to take advantage of that is by rotating it and twisting it around. Just click the mouse near the center of the graphics window and slowly drag right or left, up or down. If you have multiple buttons on your mouse, use the left button or button 1. You can also use the left and right arrow keys for small rotations. If you get lost or disoriented, use the `Views` menu to get back on familiar ground.

1.4.1.2 Identifying points

By clicking on points with the mouse (left button again), you'll be able to identify them. The label associated with each point will appear in the bottom right of the graphics area. Furthermore, the distance from this point to the last one you clicked will also be displayed.

1.4.1.3 Markers

For keeping track of which point is selected, markers can be displayed. Two markers are displayed normally. The checkbox for markers is just below the graphics area, with the pickcenter checkbox.

1.4.1.4 Turning groups on & off

Most kinemages have many different components to them, grouped together in logical ways. A protein might have one group for each subunit; or one group for mainchain, another for side chains, and yet another for hydrogens. Groups and subgroups are given names and can be made visible or hidden by the viewer — you might want to see only one subunit, or only the backbone (without sidechains and hydrogens cluttering up the view).

The groups and subgroups appear in the button pane, to the right of the graphics area. Each one has a button to turn it on or off. Groups that are on (visible) usually have a check mark or an X in there box; a blank button means the group is hidden. Many kinemages start off with some information hidden, to avoid overwhelming the reader. Always check to see if there's more information available than is being displayed!

1.4.1.5 Re-centering

You can make any point in the kinemage be the center. The center point will be in the middle of the graphics area, and the kinemage will rotate about that point. There are

several ways to set the center: you can hold the Shift key while you click the point, or use the right mouse button if you have one. You can also press the `Pick center` button below the graphics area and then click on the desired point.

Since re-centering brings a point to the center of the screen, using this repeatedly allows one to “walk” through a large structure.

1.4.1.6 Zooming in and out

KiNG allows you to zoom in to see small details in a kinemage. Use the `Zoom` slider, below the graphics area, to control how far you zoom in. You can click the mouse right or left of the knob for small movements or click the knob and drag it for larger ones. A small motion is usually all that’s needed.

For easier access, one can hold Shift and drag (or drag using the right mouse button) in the graphics window. Dragging down zooms in; up zooms out. The up/down arrow keys and mouse wheel (Java 1.4 and later only) also control zooming.

1.4.1.7 Clipping

Objects that are too near the viewer, or too far away, are not displayed; otherwise, zooming in would result in a useless superposition. The depth of the clipping “slab” can be adjusted using the slider along the bottom, or by dragging side-to-side with the right mouse button (or with the Shift key held down).

1.4.1.8 More modes of interaction

For more ways to explore the kinemage and interact with it, be sure to read about the `Navigate` tool (see 5.3 on page 19).

1.4.2 Reading the kinemage text

Exploring on your own is great, but the best guide to a kinemage is its author. Often, he or she includes a short text of a few paragraphs or pages that explains what the kinemage depicts. You can access this text using the `Show text` button, located just below the graphics area. An equivalent command is also available in the `Edit` menu.

1.4.3 Using different viewpoints

Most kinemages have one or more “views” that were selected by the author to highlight some significant feature. These views are accessible from the `Views` menu. Just click on one of the named views and the kinemage will “jump” to that view. You can then rotate it, zoom in or out, *etc.* to explore further. You can always return to the original view by selecting it again from the menu.

Kinemages without any predefined views still get an automatic “overview” view. This is a useful way to return to a known starting point if you get lost in a complicated structure.

1.4.4 Other features

The kinemage format also allows for flip-book style animations, automatic searching for points based on their name (the label that appears in the lower left when the point is clicked), and much more. There is also a rich selection of features to control exactly how the graphics are rendered. See 3 on page 13 to learn more.

Chapter 2

Input & Output

2.1 Opening a kinemage

To open a new kinemage, go to the `File` menu and choose `Open`. Browse through your file system and find a kinemage file. These files typically end in `.kin`. The new version-control convention is to name modified files `.1.kin`, `.2.kin`, *etc.*, though older kinemages that have been edited may have revisions named `.kip`, `kip1`, `kip2`, *etc.* Click the button marked `OK` and KiNG will begin loading the file. You'll see a progress bar as KiNG loads the contents of the file, and then the first kinemage in that file will be displayed in the graphics area (where the logo used to be).

You can also drag and drop kinemages into the KiNG graphics window in order to open them, but this feature is not supported for Java versions prior to 1.4. On Mac OS X machines, you can also double-click `.kin` files in the Finder or drag kinemage files onto the KiNG Dock icon to launch KiNG and open the file.

Additionally, files can be specified on the command line, as in `king -s foo.kin bar.kin`, which will load all the kinemages in those two files upon startup. The `-s` (or `-single`) flag is required so that KiNG knows not to merge the two files together.

2.2 Working with multiple kinemages

If your file has more than one kinemage, you can choose which one you want to look at from the drop box on the right, just above the buttons. You can also use `File | Open` to load additional files; those kinemages will also appear in the drop box. When you're done, use `File | Close` to get rid of the current kinemage, or use `File | Close all` to get rid of all the open kinemages.

If you save your file when more than one kinemage is open, they will *all* be written out to that file, in the order they currently appear in. This is an easy way to create multi-kinemage files, but be careful that you don't save *more* than you intended to!

2.3 Appending a kinemage

Sometimes you want to combine the contents of multiple kinemages. You might want to combine a graph of your latest sales data with some nicely formatted and labeled axes you prepared last month. Or maybe you want to combine a ribbon drawing of your favorite protein with a representation of the atomic detail at its active site. In either case, using `File | Append` will combine the contents of a new file with the contents of the currently displayed kinemage. Be careful — if the new file contains multiple kinemages, they'll *all* be merged into the current one!

This behavior can be achieved on the command line by specifying multiple files, as in `king -m foo.kin bar.kipl`, which will merge all the kinemages in those two files upon startup. The `-m` (or `-merge`) flag is optional; merging multiple files is the default behavior.

2.4 Saving kinemages

You can save kinemages using the `File | Save as` menu; these files are typically given the extension `.kin`. KiNG will try to help you by automatically appending a number to the filename so that your changes don't overwrite your original. The resulting kinemage file will be plain text that you can view and even edit by hand using any text editor (though of course you don't have to!). If you choose to do this and want use a word processor (like Microsoft Word), make sure that you load and save the file in plain text format.

Note that due to the security restrictions that web browsers place on Java applets, saving will never be possible when KiNG is running inside a web browser.

2.5 Printing kinemages

You can use `File | Print` to send the image in the graphics area to your printer. The image will fill as much of the page as possible without distorting it. The relative size of the elements will be exactly the same as on screen. Among the consequences of this are that an image printed from a small graphics window will have thicker lines when printed than will the image when printed from a larger graphics window. Don't worry about this too much; just remember printing is WYSIWYG (what-you-see-is-what-you-get). If it looks right on the screen, it should look right on the paper! Some images will fit better in landscape mode than portrait mode; this decision is left up to the user.

Printing should work even when KiNG is running in a web browser, although the user will generally be asked for permission first.

2.6 Exporting kinemages in other formats

Several facilities are provided that can help get data out of kinemage format and into other forms, either for making figures for publication or for further processing. Due to

security restrictions placed on applets, the export features are unavailable when KiNG is running in a web browser.

2.6.1 Exporting bitmapped images (JPEG, PNG)

The `File | Export` menu allows one to save the current graphics image as a standard image file. Image export requires that you have Java 1.4 or newer; otherwise, an error message will appear. Several image formats are supported, including JPEG and PNG; the format can be selected from the export dialog box. These images are very useful for creating web pages, PowerPoint-style presentations, *etc.* For high-quality publication graphics, however, you'll want to use a vector-based format like PDF.

2.6.2 Exporting vector graphics (PDF, PostScript, *etc.*)

Rather than sending the image to the printer, it can be captured for inclusion in a publication or later manipulation in a graphics program like Adobe Illustrator. Note that there are several relevant options under the `Display` menu, particularly `White background` and `Monochrome`.

All platforms can generate PDF files using the `File | Export` menu. This is the simplest and best option for almost any use. "PDF" stands for Portable Document Format, the successor to PostScript as the standard for vector graphics. You can learn more about PDFs at <http://www.adobe.com>. It does require the (free) iText PDF library from <http://www.lowagie.com/iText/>, which is distributed with KiNG.

If for some reason you don't want to use PDF export, it is also often possible to hijack the print output into a file. For instance, with Macintosh OS X, both PostScript and PDF output are supported directly from the Print dialog. Under Linux, choosing `Print to file` from the Print dialog will generate a PostScript file, which can be converted many other formats using *e.g.* Ghostscript tools like `ps2pdf` (PDF) and `ps2epsi` (EPS, Encapsulated PostScript). Under Microsoft Windows, things don't seem to be as straightforward, but one possibility is to install the generic PostScript printer drivers from Adobe and then direct this "virtual printer" to `FILE` (rather than, *e.g.*, `LPT1`). Your mileage may vary; I'd be interested in hearing about better ways to do this from any Windows experts out there.

2.6.3 Exporting as XML

This feature now lags far behind the rest of the program in functionality; it may not work at all. If you need this capability, you are encouraged to contact the author and encourage on-going development.

You can export kinemages in XML format using the Kinetic Image Markup Language by choosing `Kin-XML` from the `File | Export` menu. We recommend giving these files the extension `.xkn` or `.xml`. At this time, KiNG does not read these files, nor do other kinemage viewers. Also, they may not include all of the information that would be present in a traditional kinemage file. However, for people who would like to operate on the data from a kinemage without having to write a parser for the kinemage

format, we expect this will be useful and convenient. Translation from the modified XML back to kinemage format is left as an exercise to the reader ;)

2.6.4 Exporting as VRML

KiNG has rudimentary abilities to export its 3-D primitives in VRML97 (a.k.a. VRML 2.0) format. At present, only dots and balls are exported, and they are both rendered as spheres. This feature was intended to facilitate the creation of models for rapid prototyping systems. As with XML export, contact the author if further development of this feature would be useful to you.

Chapter 3

Advanced kinemage reading

3.1 Finding points by name

Every point in a kinemage has an associated identifying label, which appears in the graphics area when the point is clicked on. You can find one or more points by searching through those labels for a word or phrase using the `Edit | Find point` dialog. When you press `Search`, KiNG will center the view on the first point that matches your criteria (you may need to zoom in/out to see it appropriately). `Edit | Find next` will then jump to the next matching point, until all matches are exhausted.

3.1.1 Whole word searches

This is the easiest-to-use of the search options, and usually produces the desired results. You can enter one or more words or numbers in the search field (separated by spaces), and KiNG will find all the points that contain *all* of those words, in any order. A search for “val 17” would find “17 A val cb” but not “valine 117”.

3.1.2 Substring searches

This works like whole word searches, but will even find points that have the search terms embedded in a larger word or number. In this case, a search for “val 17” *would* find “valine 117”. This often produces extraneous results but may occasionally be useful.

3.1.3 Glob (simple regex) searches

This search is done with a simple “regular expression”, as is often used for specifying file names on the command line. A star (*) matches any group of zero or more characters, and a question mark (?) matches any single character. Notice that the search is treated as a single term, rather than multiple words — the pieces must be in the correct order. Thus a search for “val*17” would find “val17”, “val 17”, and “valine 117”, among others; but would *not* find “17 val”.

3.1.4 Perl5 regex searches

This search is like the simple regex search but uses the full syntax of Perl 5 regular expressions, as implemented by the `gnu.regex` library. (I'm no expert, but it seems to be a very complete and official implementation. All but the most esoteric features are available.) Regular expressions are a very involved subject, and many books and on-line references are available for the interested reader.

3.1.5 Tips for faster searches

Remember that KiNG searches through *all* visible points to find ones matching your criteria. Turning off (*i.e.*, making invisible, hiding, unchecking) large groups that you're not interested in will skip searching those groups. Since all the varieties of search are implemented internally with regular expressions, they are relatively computationally expensive. A search through a large kinemage may take several seconds.

3.2 Viewing animations

Kinemages often include animations. An animation in this sense is not a movie, but more like a flip-book, where similar images are aligned and displayed one at a time, in a series of discrete frames. If a kinemage contains animation(s), there will be forward and reverse buttons for the animation located below the checkboxes for groups and masters.

3.3 Controlling presentation: The Display menu

The `Display` menu offers several options for controlling how the kinemage is rendered. Of particular interest is the `Perspective` option. By default, KiNG renders objects with orthographic perspective; objects near the viewer are no larger than those far away. This is the preferred mode for viewing macromolecular structures and many 2-D graphs and figures. However, for geometrical objects and other cases where the eye expects perspective, enabling this option will result in a much more natural-looking image.

There are also several ways of controlling the coloring of the points. Each point may have its own color, and several "aspects" as well. For example, a map might be colored by the aspects of temperature, elevation, and annual rainfall; one could then choose which of these colorings to apply.

The first level of grouping above the individual point is the list; every point belongs to a list. Points that don't have a color specified take their color from the list, but there are times when one might want to suppress the individual colors and color points by the color of the list they belong to. This option is available as well.

3.3.1 Stereo

Upon request, KiNG will render the kinemage as a stereoscopic pair of images. The two views are very nearly the same, except that one is slightly rotated with respect to the other. If you can get one eye to look at each image, you can fool yourself into seeing additional depth information. Stereo can be either “cross-eye” or “wall-eye”; the former is somewhat easier to learn, but the latter is more comfortable for long periods of time.

To see cross-eye stereo, cross your eyes and then look at the screen without refocusing. You should see 4 identical (though blurry) images. Relax your eyes slightly, and the center two will overlap. If you can focus on this phantom central image, you’ll be seeing in stereo. It may help bring the image into sharp focus to rotate the kinemage slightly using the mouse.

If you’ve got KiNG set for wall-eye stereo and your eyes set for cross-eye (or vice versa), you will see a stereoscopic image, but the parts that should be in back will be in front, and it will rotate the wrong direction when you move the mouse. Change one or the other to get a more reasonable image.

Incidentally, although KiNG doesn’t support multiple simultaneous views of the same kinemage, you can simulate a pair of orthogonal views by setting the stereo separation to 90 degrees in `Edit | Configure KiNG`. Of course, the views no longer form a stereo image, but they’re useful in another way. Particularly applicable for “info-vis” kinemages, you can examine (for instance) the x-y plane and the y-z plane at the same time using this trick. It pairs well with the 90-degree rotations plugin (5.15).

3.4 Master buttons

Not all the buttons to the right of the graphics control groups and subgroups of points; some are “masters.” The master buttons sit below the others, separated by a spacer. When activated, a master turns on all the groups it controls; when deactivated, it turns them all off. The effects are only momentary; the group can be turned on or off directly regardless of the state of the master(s) that control it.

A single group can be controlled by multiple masters. Note that the “off” state of a master is dominant in this case: a master will always turn off the groups it controls, but will turn them on only if they are not also controlled by another master that is already off. Since the buttons of the individual groups, subgroups, and lists are sometimes hidden, one can generate a variety of patterns by turning the masters on and off in specific patterns.

Chapter 4

Kinemage authoring: Using KiNG to edit a kinemage

Kinemage files are stored as human-readable, plain-text files. They're also designed to be easily edited by human beings, using a text editor like Notepad (Windows), TextEdit (Mac), or vi (Unix). You can also use a word processor like Microsoft Word, but you have to be careful to save as plain text (.txt) rather than formatted text (.doc and others). A description of the kinemage file format is distributed with KiNG as a separate document from this manual.

4.1 Merging kinemages together

The most basic sort of editing is to combine two kinemages into one. For this, simply use the `File | Append` command (see 2.3 on page 10).

4.2 Editing text

The text of a kinemage is often critical for clarifying and amplifying its meaning. It's analogous to the caption that accompanies a printed figure. You can edit the kinemage text in the same window that you use for reading it (just press the `Show text` button).

4.3 Editing views

A simple editing tool is `Views | Save current view`, which records the current orientation and position of the kinemage as a new view in the `Views` menu. Creating a series of meaningful, clearly labeled views is a great way to make a kinemage more informative. You can delete, rename, and rearrange views using `Views | Edit saved views`.

4.4 The hierarchy editor

One of the goals of KiNG is to enable simple, visual editing of most parts of a kinemage. Many of the editing commands are activated using a tree-like display of the hierarchical kinemage structure, which will resemble the layout of buttons.

The structure of the kinemage can be rearranged by cutting, copying, and pasting elements; creating new elements and deleting unneeded ones; and reordering elements (using the `Up` and `Down` commands). Play with these commands, and their operation will soon become obvious. Elements can even be cut out of one kinemage and pasted into another!

Also, the properties of individual elements can be adjusted, which allows them to be renamed. What other properties are available depends on the level of the hierarchy (kinemage, group, subgroup, or list). Each element can also be toggled on and off, even if it doesn't have a button visible in the button pane.

Using the hierarchy editor effectively depends on a decent understanding of the kinemage format. If you're unfamiliar with kinemages, reading the kinemage format reference may be very helpful to you.

Chapter 5

The Tools

5.1 Understanding the Tools and Plug-ins

The `Tools` menu has a variety of tools and plug-ins for interacting with the kinemage. Many of these are highly domain-specific — tailored to doing structural biology, for example. Each tool “takes over” the mouse, assigning specific meanings to the various kinds of clicks and drags. Normally, the familiar `Navigate` tool is active, so mouse motions result in the sort of rotations, pans, and zooms that most users are accustomed to.

Plug-ins, on the other hand, just offer additional functionality that doesn’t change what the mouse does. Because of this, you can have several plug-ins active at once, but only one tool.

The tools menu also has some other options that are related to how mouse clicks and drags are interpreted, which are discussed below. The tools and plugins listed in the menu can be rearranged, grouped into submenus, or hidden entirely by using the `Tools | Customize` dialog box, which is also accessible from `Edit | Configure KiNG`.

5.1.1 Extra measurements

In addition to tracking the distance between the last two points, clicking on points to identify them can track the angle between the last three points and the dihedral angle between the last four. When these measurements are active, the `Markers` option will display four markers instead of two.

5.1.2 XYZ coordinates

Likewise, KiNG can display the original, unrotated coordinates of the point. This is sometimes helpful when the kinemage is a graph or plot of some data, and the position has some absolute meaning. The display of this information can be enabled in the `Tools` menu.

5.2 Using KiNG with a multi-button mouse

In KiNG, even a one-button mouse is sufficient to access all of the available functions. However, it has also been designed to take full advantage of a three-button wheel mouse. The primary function of every tool is accessed by clicking or dragging with the left (or only) mouse button. This button is referred to as “Normal” in the command reference charts.

Other functions can be accessed either by holding down keyboard keys at the same time, or by using one of the other mouse buttons. Holding the Shift key is equivalent to using the right mouse button, and holding the Control key (often written Ctrl) is equivalent to using the middle mouse button. A few tools assign some function to a mouse action with both the Shift and Control keys held down. In this case, you can get the same effect when dragging by depressing both the left and right mouse button. Because of the difficulty of clicking two buttons at once, however, this shortcut does not apply to Shift+Ctrl+Click.

Some tools also use the up & down arrow keys on the keyboard; these have the same effect as using the scroll wheel of a wheel mouse. Once again, these may be combined with the Shift and/or Control keys to give access to more functions. Note that the mouse wheel is never active when running in a Java 1.3.x virtual machine; Java 1.4 or later is needed to take advantage of this control.

5.3 Navigate: Exploring in 3-D

The Navigate tool encompasses all the usual modes of interacting with a kinemage. This is the tool that is active when KiNG is launched, and is probably the only tool many people will ever use. See 1.4.1 on page 6 for an introduction to using the Navigate tool to get around a kinemage. There are also a few more advanced modes of movement which are described below.

5.3.1 Z-rotation (“pinwheel”)

Clicking and dragging (with the left mouse button) near the top of the graphics area will cause the kinemage to spin around the Z axis like a pinwheel, rather than the more conventional sort of rotation. This is sometimes useful for putting something right side up.

5.3.2 Translation (“flatland”)

Holding Control while dragging (or dragging with the middle mouse button) allows one to slide the kinemage around in the plane of the screen. Dragging at the top of the screen, as for z-rotation, slides the kinemage in and out of the plane of the screen. (Note: enabling perspective in the Display menu is *very* helpful when translating in and out of the plane of the screen.) This sort of motion is sometimes called “panning” or “flatland,” and can be made the default mode of movement by selecting Tools | Flatland.

5.3.3 Command reference

Mouse clicks	
Normal	Mark and identify point; make measurement (pick)
With Shift	Center on selected point (pickcenter)
With Ctrl	-
With Shift+Ctrl	-

Mouse drags	
Normal	Rotate around X and Y axes; Z-rotate (pinwheel) near top of screen
With Shift	Adjust zoom (up/down); Adjust clipping (left/right)
With Ctrl	Translate in X-Y plane (flatland); Z-translate near top of screen
With Shift+Ctrl	Rotate around Y axis only

Mouse wheel / Up & Down arrow keys	
Normal	Adjust zoom
With Shift	Adjust clipping
With Ctrl	-
With Shift+Ctrl	-

5.4 Move Points: Remaking the kinemage

This tool allows you to click on individual points and drag them around to new positions. Dragging them with the mouse moves them in the plane of the screen. Using the mouse wheel or up & down arrow keys moves them in and out (this is easier to see with Perspective enabled and Stereo on). A kinemage may have several “points” at the same location in 3-D. Under normal conditions, this tool will move them all together, so that lines stay connected and everything behaves just as you would expect. However, you can also use Ctrl+Drag to pick apart overlapped points and separate them from each other. You will need to activate the **Tools | Superpick** option to edit unpickable points.

5.4.1 Command reference

Mouse clicks	
Normal	Mark and identify point; make measurement (pick)
With Shift	Center on selected point (pickcenter)
With Ctrl	-
With Shift+Ctrl	-

Mouse drags	
Normal	Move all overlapped points together in X-Y (on a point); X-Y and Z-rotation (otherwise)
With Shift	Adjust zoom (up/down); Adjust clipping (left/right)
With Ctrl	Move top-most point only in X-Y (on a point); X-Y and Z-translate (otherwise)
With Shift+Ctrl	Rotate around Y axis only

Mouse wheel / Up & Down arrow keys	
Normal	Move all overlapped points together in Z
With Shift	Adjust clipping
With Ctrl	Move top-most point only in Z
With Shift+Ctrl	-

5.5 Edit Properties: Changing colors and more

This tool is just like Navigate, except that picking a point opens the editing window for that point (or that point's list for Ctrl+Click). You will need to activate the **Tools** | **Superpick** option to edit unpickable points.

5.5.1 Command reference

Mouse clicks	
Normal	Pick point and edit its properties
With Shift	Center on selected point (pickcenter)
With Ctrl	Pick point and edit list properties
With Shift+Ctrl	-

Mouse drags	
Normal	Rotate around X and Y axes; Z-rotate (pinwheel) near top of screen
With Shift	Adjust zoom (up/down); Adjust clipping (left/right)
With Ctrl	Translate in X-Y plane (flatland); Z-translate near top of screen
With Shift+Ctrl	Rotate around Y axis only

Mouse wheel / Up & Down arrow keys	
Normal	Adjust zoom
With Shift	Adjust clipping
With Ctrl	-
With Shift+Ctrl	-

5.6 Draw New: Reworking the kinemage

The Draw New tool provides a variety of simple tools for creating new objects in the kinemage or removing existing ones on a point-by-point basis. Remember that you can use the Edit Properties (5.5) and Move Points (5.4) tools to further customize your creations in terms of color, width / radius, point ID, position, *etc.*

Draw line segments Simply draws a line between the first point picked and the second. Every pair of picks forms a new line. Lines can be shortened from their natural length (or lengthened, using negative numbers), which is sometimes useful for making illustrations.

Draw balls Places a small ball at each point picked with the mouse.

Draw labels Creates a label at the picked point, with its text taken from the picked point's ID. The label text can be changed using Edit Properties.

Draw dots Creates a dot at each point picked with the mouse.

Draw dotted lines Like drawing ordinary lines, except a string of dots is created instead of a single line. The number of dots is configurable. This can serve as a "template" for constructing more complex dot-dash patterns when used with line drawing and prune.

Draw curved arc Draws an arc from the second point picked to the third one, with the arc curving toward the first point picked. The user specifies how many degrees out of a circle will be used to create the arc, so small numbers give flat arcs and large numbers give exaggerated ones. The arc can also be shortened by a few degrees so it doesn't quite touch its endpoints, and a four-pronged arrowhead can be added.

Draw triangles Draws a triangle for each set of three points picked. Triangles can also be shrunk (values between 0 and 1) or grown (values greater than 1). A value of zero will make an infinitely small triangle; a value of one will give a triangle that just touches the three points.

Prune one point Removes the single point picked with the mouse. In the case of polylines and triangle strips, it will stop things from being drawn that depend on the removed point. That is, lines drawn to and from the point will be removed, and all triangles involving the point will be removed. Sometimes kinemages have multiple points that overlap in the same spatial location, so it may take multiple clicks to remove all the objects at a particular point in space.

Punch a polyline Removes all the line segments in a particular *polyline* (a series of lines drawn head to tail). This is sometimes useful with vectors and triangles; for other things, it behaves like prune.

Auger a region Removes all points that fall under the giant eraser. The eraser is drawn as a large circle that follows the mouse around the graphics area. Auger operations cannot be undone, so save your file first and click carefully.

Spherical crop Removes all points that fall more than a specified distance away from the picked point. Only visible points are cropped. Crop operations cannot be undone, so save your file first and click carefully.

New subgroup Kinemage elements created by each drawing option are placed into their own list, and all of those lists are placed in one subgroup under the “New group” group created by this tool. Creating a new subgroup starts a fresh list for each option above. This is a good way to separate out the different objects you’re drawing. New subgroup can’t be undone, but it’s pretty harmless.

Undo The Undo button undoes the last drawing action, with a few exceptions (mentioned above). Undo depth is unlimited, subject to memory constraints. Thus, for kinemages that aren’t too large you can often undo all the drawing operations you’ve performed since loading the kinemage.

5.7 Dock 3-on-3: Geometric construction

The three-point docking tool is useful for constructing geometric shapes and figures out of existing pieces in kinemage format. As you start picking points with the mouse, they will be labeled with numbers: first three points in the reference frame, then three in the mobile frame. When you’re ready to apply the docking transformation, turn off groups that should remain in place and leave visible those that should move. Then press the **Dock** button. The first points will be superimposed exactly, the 1-2 axes will be aligned (so that the mobile “points in the direction of” the reference) and the final points are used to determine rotational position (dihedral angle) about the 1-2 axis.

If you’d like to dock several of the same object with respect to each other, remember you can use the copy and paste commands in the hierarchy editor to create duplicate objects.

5.8 Least-Squares Docking: Getting the best fit

The least-squares docking tool is useful for matching up two objects that are similar but not quite the same. As you start picking points with the mouse, they will be labeled with numbers, defining the Reference frame. Once you’ve selected something to dock onto, you should choose the Mobile frame and add an equal number of points to it. The order matters: 1 will match with 1, 2 with 2, and so on. When you’re ready to apply the docking transformation, turn off groups that should remain in place and leave visible those that should move. Then press the **Dock** button. The matched points will be positioned so as to minimize the sum of the squares of their separation (thus the phrase “least squares”).

If you’d like to dock several of the same object with respect to each other, remember you can use the copy and paste commands in the hierarchy editor to create duplicate objects.

5.9 C-alpha Hinges: Protein chirpraxis

The Hinges tool is used to adjust segments of protein backbone without disturbing the surrounding structure. It allows you to select a region of backbone that joins two alpha carbons, and then rotate that segment of backbone around an axis drawn between those C-alphas. Using Hinges requires that `chirpraxis.jar` be present in the same folder as `king.jar`.

Create a hinge by control-clicking the alpha carbons that act as its endpoints or anchors. To use the dial control, click and drag the pointer to the desired value. For finer control you can shift-drag along an imaginary slider (this behavior is somewhat like the virtual dials in O). To reset the dial to its starting value, double click the dial face. The dial can also be adjusted from the graphics window using the mouse wheel or arrow keys; see below.

The Hinges panel provides feedback on the geometric quality of the current model, displaying residues names, deviation of the tau angle (N-CA-C) from ideality, and the position of the residue on the Ramachandran plot (phi, psi, and favored/allowed/outlier). Deviant geometry is highlighted in red.

The “Karplus” field is an alternative measure of deviation in the tau angle, based on data in P. A. Karplus’ 1996 “Hidden Strain” paper (Protein Science 5:1406). There he calls the angle tau3, and claims that its average value varies substantially depending on the value of backbone angles phi and psi. The meaning and usefulness of a deviation from this number is still under investigation.

Hinges has not yet been published. When it is, a citation will appear here.

5.9.1 Command reference

Mouse clicks	
Normal	Mark and identify point; make measurement (pick)
With Shift	Center on selected point (pickcenter)
With Ctrl	Select anchor for hinge (on a C-alpha); clear current selection (elsewhere)
With Shift+Ctrl	-

Mouse drags	
Normal	Rotate around X and Y axes; Z-rotate (pinwheel) near top of screen
With Shift	Adjust zoom (up/down); Adjust clipping (left/right)
With Ctrl	Translate in X-Y plane (flatland); Z-translate near top of screen
With Shift+Ctrl	Rotate around Y axis only

Mouse wheel / Up & Down arrow keys	
Normal	Adjust dial (angle of rotation)
With Shift	Adjust clipping
With Ctrl	Adjust zoom
With Shift+Ctrl	-

5.10 Sidechain Rotator: Refitting protein models

The Sidechain Rotation tool is useful for doing interactive refitting of protein models in conjunction with the Hinges tool and the model manager. Use Ctrl+Click (a.k.a. middle-click) to select a sidechain to rotate, then pick from a list of predefined rotamers or set the angles by hand using the dials. The rotamericities of the current sidechain is monitored in the bottom right corner; it indicates how frequently (if ever!) the current conformation is found in well-determined structures.

To use the dial control, click and drag the pointer to the desired value. For finer control you can shift-drag along an imaginary slider (this behavior is somewhat like the virtual dials in O). To reset the dial to its starting value, double click the dial face.

Sidechain Rotator and the Hinges tool play well together: you can use both on the same residue(s) at the same time. It's often easiest to establish which sidechains will be rotatable before beginning to move the backbone, but it's possible to establish the moving parts in any order.

5.11 Sidechain Mutator: Redesigning protein models

The Sidechain Mutation tool is useful for doing interactive refitting of protein models in conjunction with the Hinges and Rotator tools and the model manager. Use Ctrl+Click (a.k.a. middle-click) to select a sidechain to mutate, then pick from a list of known amino acid types. If you select histidine, you will also be prompted to choose a protonation state.

Sidechain Mutator plays well with the other tools, but you cannot mutate the model while any part of it is mobile ("molten"). Thus, it's often easiest to make mutations first, and then refit the new sequence.

5.12 Model Manager: Editing a macromolecular model

This facility is for doing molecular modeling based on some starting model, usually a PDB file. The Model Manager handles opening and saving these files, and is required for the operation of the following tools:

- C-alpha hinges
- Sidechain rotator
- Sidechain mutator

The model manager also tracks the changes made to the model and allows near-unlimited undo. In addition, it provides access to dynamic visualizations, like Probe dots and NOE constraints. Using this feature requires that your OS can find Probe – *i.e.*, that either Probe resides in the same directory as `king.jar` and is named either `probe` or `probe.exe`; or that Probe is somewhere on your PATH and is named `probe` or `probe.exe`. The same is true of `noe-display`.

There are several special symbols that can be inserted into the Probe and NOE command lines. Their meanings are as follows:

{pdbfile} The fully-qualified name of the “base” PDB file; *i.e.* the one with all changes except the currently molten ones. (Those are piped in via standard input.)

{molten} The list of molten residues, separated by commas: 1, 2, 3, ...

{center} The coordinates of the current center of view, in real space: x, y, z. This can be used for the *within distance* of x, y, z selection statement. Note that visualizations aren’t automatically updated when the center of view changes.

5.13 Electron Density: Visualizing maps

This plug-in is for viewing electron density maps while exploring kinemages of crystal structures. (If that doesn’t mean anything to you, then you probably don’t need this plugin.)

Choose **Open** from the **Tools** menu in order to open a map file. Supported formats include X-PLOR (ASCII, not binary), O (DSN6 or Brix), and CCP4 (mode 2, the only one in common use).

Each map opens a new control window, which allows adjustment of its extent, color, and level. The segment of map that is visible at any given time is centered in the current view; when the view changes, the portion that is visible will automatically be updated.

Any dynamic segment of map can be “captured” as part of a static kinemage; just use the **Export** button to make the currently visible map segment part of the current kinemage. When you’ve finished with a map, be sure to **Discard** it to free up the memory it consumed.

If you don’t have an electron density map for the structure you’re interested in, you can try looking at the Uppsala Electron Density Server (<http://fsrv1.bmc.uu.se/eds/>). They offer standard maps for many of the structures deposited in the Protein Data Bank.

Maps can’t be loaded from the local filesystem when KiNG is running as an applet due to security restrictions. However, you can use the **XMAP** or **OMAP** parameter along with the **<PARAM>** tag to load a (single) map from a URL. For example:

```
<PARAM name="omap" value="http://example.com/electron/density/my-protein.dsn6.gz">
```

You can also use the **EDMAPBASE** and **EDMAPLIST** parameters to allow the user to select and load a map. **EDMAPBASE** specifies a path to the maps relative to the current document base URL. **EDMAPLIST** is a space-separated list of filenames that can be loaded from that path. Users can also enter and modify URLs directly, though obviously this isn’t very convenient.

5.14 RNA Maps: Finding the phosphates

Authored by Vincent Chen (vbc3@duke.edu)

This tool (still under development) was designed to aid users in locating potential phosphate positions in the electron density maps of nucleic acids. Similar to the existing electron density viewing plug-in, this tool asks the user to open a map file, and opens a control window containing many of the same controls as the electron density plug-in. In addition to these controls, it has a toggle button to activate/deactivate the "poly picking" feature and a color selection list. When active, if the user left-clicks on a point in the kinemage, the polyhedron containing that point will be highlighted in the color selected. Next, the tool searches through the map to find the highest electron density value within that selected polyhedron, and places a marker point on that spot, showing an approximate position for the phosphorous.

5.14.1 Current Issues

This tool does not differentiate between a point in the electron density and a point on the actual structure. Clicking on the structure with the poly picking tool active can result in the program searching through the whole structure, which can take a very long time. Be sure to click carefully, and to limit the polyhedra to be selected to a reasonable size (i.e. have the sigma level set high enough that the polyhedra are about the size of a phosphate). Also, once the first polyhedron has been selected, moving the electron density around and selecting a polyhedron may result in an error. If this happens, the program will have to be restarted in order to select a polyhedron not in the initial set.

5.15 90 Degree Rotations: Seeing precisely

The 90 Degree Rotations plugin provides a simple way to turn your model by 90 degrees around any of the three Cartesian axes. It also provides a shortcut back to the standard kinemage orientation: looking straight down the Z axis from the positive end toward the negative one, with positive X to the right and positive Y at the top of the screen.

This plugin is particularly useful in combination with a trick for setting up simultaneous orthogonal views of a kinemage. Read about it in the section on stereo graphics (3.3.1).

5.16 Solid Object Drawing: Just for fun

The solid objects plugin is a fun helper that shows what a wide variety of shapes and forms can be constructed from a clever combination of kinemage primitives.

5.16.1 "Lathe" tool

The lathe tool takes a single polyline and sweeps it out around an axis to create a polygonal object. One strip of 64 triangles is created for every line segment. This tool

is ideal for creating anything with an axis of symmetry: bottles, vases, lamps, simple cylinders, and so on. The standard axis of rotation is the Y-axis, with rotation centered at the origin, so keep this in mind when drawing a half-profile to use with this tool.

Chapter 6

Configuring KiNG

By choosing `Edit | Configure KiNG`, one can adjust several aspects of KiNG's behavior and appearance, such as font sizes, stereo settings, and whether or not certain warnings are issued. The configuration dialog also allows for reorganizing the `Tools` menu to suit your own work habits. Preferences may be saved to disk, where they are stored in a simple text file named `.king_prefs` in the user's home directory. There may be some settings accessible only through this file; that is, they cannot be edited from the graphical interface. Nonetheless, pressing `Reset to defaults` will restore them to their standard values.

Note that due to security restrictions, configurations cannot be saved when KiNG is running as an applet. However, the web page creator may provide a custom configuration file in the same format as the one saved by KiNG the application, thereby altering the default behavior for all visitors to the website. If you create a preferences file named `MyKingPrefs.txt` and place it in the same directory as `king.jar` and your HTML file, add something like this to the `APPLET` tag of your webpage:

```
<param name="king_prefs" value="MyKingPrefs.txt">
```

Chapter 7

Launching KiNG

KiNG runs both as a stand-alone application, and as an applet that can be included in web pages. In any case, KiNG requires a Java Virtual Machine (JVM), version 1.3 or higher. You can get Java from <http://java.sun.com>.

7.1 Running KiNG as an application

How you launch the KiNG application will depend on what operating system (Windows, Mac OS X, Linux, *etc.*) you're using. With Windows and the Mac, you can usually just double-click on the `king.jar` file to start KiNG.

On all operating systems, you can type

```
java -jar king.jar [-merge | -single] [file1 file2 ...]
```

All the files listed on the command line will be merged together into one kinemage,, unless the `-s` flag is included, in which case all the files will be opened as separate kinemages.

7.2 Making KiNG an applet in a web page

KiNG can also be included as a web page applet. The following HTML code is a simple example that uses the `<APPLET>` tag, which will work with browsers using a recent JVM. Older browsers may need `<OBJECT>` or `<EMBED>` tags; more information on this is available from Sun Microsystems, Inc.

```
<applet code="king/Kinglet.class" archive="king.jar" width=300 height=150>  
<param name="kinSource" value="some_file_name.kin">  
</applet>
```

Just put all the jar files, including `king.jar`, in the same directory as the HTML file. Users who visit the page will see a 300x150 KiNG logo in the web page, along with a

floating KiNG window that looks very much like the stand-alone application. However, due to security restrictions imposed by the browser environment, some functions (*e.g.*, saving files) will be disabled.

Note that the `code` property really must have the value `king/Kinglet.class`, *even though `king.jar` is not in a sub-directory called `king/`*. This is the most common problem that people have when trying to run KiNG as an applet. If you did place `king.jar` somewhere else, that path should precede the jar file name in the `archive` property instead.

It is possible to run KiNG in two other applet modes to achieve a slightly different effect. First, the large KiNG logo can be replaced with a small one that serves as a launcher button. Thus, loading the main window is deferred until the user clicks the button, at which time the main window appears and the kinemage is loaded. Below is sample HTML for this effect. Note the smaller width and height, to account for the small size of the button.

```
<applet code="king/Kinglet.class" archive="king.jar" width=60 height=21>
<param name="mode" value="launcher">
<param name="kinSource" value="some_file_name.kin">
</applet>
```

Second, the applet can be embedded in the web page (rather than floating in its own window), by placing this line inside the `<applet>` tags instead:

```
<param name="mode" value="flat">
```

One also probably wants to specify a larger width and/or height, possibly as a fraction of the page size (*e.g.* 95%). Be warned that using KiNG this way may not work well in some browsers; test your pages thoroughly.

Some Tools and Plugins may define their own `<PARAM>` tags, which will be described in their documentation.

Chapter 8

Additional resources

8.1 Included manuals

In addition to this User's Guide, KiNG may be accompanied by a guide to the kinemage file format. Kinemage files are simple text files, so that anyone can create kinemage illustrations by hand. This is especially important to fields where no automated tools for kinemage creation yet exist.

8.2 Included kinemages

Under the `Help` menu, KiNG has several built-in kinemages that demonstrate various capabilities of the graphics system. The palette is particularly useful to kinemage authors when they are designing color schemes.

8.3 External documentation

The best resource for learning more about kinemages is the Richardson lab website, <http://kinemage.biochem.duke.edu>. Many other resources exist; hopefully, they will be documented here in the future.

8.4 Bug reporting and contact info

Ian Davis, the author of KiNG, may be reached via email at <mailto:ian.davis@duke.edu>. *Please*, do not hesitate to report bugs and problems with KiNG — your input can only improve the program.

Chapter 9

Copyright & acknowledgments

9.1 Copyright

The KiNG program and all its associated original resources and documentation are copyright (C) 2002-2004 by Ian W. Davis. KiNG makes use of the `gnu.regex` library, which is copyright (C) by Wes Biggs, and of icons copyright (C) by Sun Microsystems provided for use with Java programs.

9.2 Licenses

KiNG is free software available under the terms of its own BSD-style license (see A on page 35). The source code and new versions can be downloaded from the Richardson lab website, <http://kinemage.biochem.duke.edu>. The `gnu.regex` library is covered by the GNU Lesser General Public License (LGPL). In accordance with that license, the full source of the `gnu.regex` library is available from its website at <http://www.cacas.org/java/gnu/regex/>. The `iText` library is dual-licensed under the LGPL and the Mozilla Public License (MPL). `iText` is available from <http://www.lowagie.com/iText/>. Many of the icons are the property of Sun Microsystems and have their own license; they are available from <http://developer.java.sun.com/developer/techDocs/hi/repository/>.

All license documents are provided in the downloaded KiNG bundles and are found in the `doc/` directory. Additionally, the KiNG license appears in the Appendix (see A on page 35).

9.3 Acknowledgments

I owe an enormous debt of gratitude to many, many people for making this program possible. First and foremost, I thank David and Jane Richardson, who are my bosses and mentors, and who developed the kinemage concept, the file format, and most of the features found in KiNG — my contribution was only the Java implementation. Second,

I am grateful to the other members of the Richardson lab, who have supported and encouraged me in developing KiNG, providing invaluable insight into how to improve the program.

KiNG is free software built on free software. I can't hope to acknowledge all the authors of all the software that has been used to create KiNG, but I can mention a few of the most prominent: Sun Microsystems, the creators of the Java language and libraries; the gnu.regexp project, which provides regular expression support to KiNG; the LyX document processor, used for writing the documentation; jEdit, a fantastic programmer's text editor written entirely in Java; and of course RedHat and the entire Linux movement, for providing what is arguably the best OS available today.

9.4 Revision status

This manual was last updated 18 May 2004 by IWD for KiNG version 1.26.

Appendix A

KiNG License

A.1 What this license applies to

This license applies to everything in this project that is the original work of the copyright holder(s) and contributor(s), including but not limited to the source code, binary executables, artwork, and documentation. This distribution includes certain third-party libraries and resources which are not covered by this license, and which are governed by their own license terms. See documentation for more details.

A.2 The KiNG License

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