The Extratools manual

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Chapter 1

The Tools

1.1 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.

1.2 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.

1.3 RNA Maps: Finding the phosphates

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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.

1.3.1 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 selected a polyhedron not in the initial set.

1.4 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 in the KiNG manual.

1.5 “Lathe” tool: Just for fun

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

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 2

Editing kinemages

Several new tools have been created that allow kinemages to be more easily edited without having to go back to the original PDB and creating a new kinemage.

2.1 Recoloring

KiNG now has the ability to easily recolor kinemages. This tool was designed to specifically recolor protein structure kinemages; however, it can probably be used to recolor other kinds of kinemages as well. It allows specific regions of a structure to be recolored. For example, a specific amino acid, a particular alpha helix, or a whole subunit can be highlighted. This tool can also create a table of the amino acids in a structure.

The control panel for this tool has a number of options. The top line contains the color options, the second line contains the area of effect options, and the third line contains info boxes about what you are coloring and some extra control options. Most of the coloring is activated by clicking on the structure. It is important to note that this tool only recolors lists and subgroups, so depending on your kinemage, it is possible to color the sidechains separately from the backbone. Also, this tool only colors by point color.

Usage tip: There seems to be some issues with serine sidechains not being able to be colored. To work around this, try turning on the "Pick Objects" option in the Tools menu, and click directly on a bond in the sidechain.

2.2 Kinemage Fudging

The KinFudger tool now allows distance and angles between points to be easily adjusted. This is especially useful in modifying bond distances, angles, and dihedrals in macromolecular structures.

The control panel is simple, consisting of options for the parameter you wish to adjust, whether you want to move only one point (and all attached single points–I use

this to move an atom and its attached hydrogens), and a button to export your kin to PDB.

2.2.1 Adjusting bond distances, angles, and dihedrals

In order to adjust a parameter, select the parameter you wish to adjust and click on the kinemage points you want to adjust, in order as if you were doing measures. By default, the tool will move the last point you clicked on, plus all the points connected to that point excluding the points "behind" the points you clicked. So for example, if you had a A-B-C-D connection, and you were adjusting the distance between B and C, and you clicked on B first, then C, then the program would move C and D. Likewise, if you clicked on C first, and then B, the program would move A and B. Naturally, the connectivity finding algorithm I use gets confused if you are adjusting with a cyclic structure, so be careful in that situation.

An interesting use I discovered about this tool is that you can use the distance adjusting to do a one-point docking of structures to close gaps.

2.2.2 Exporting to PDB

The KinFudger also includes an export to PDB functionality. As long as your kinemage PointIDs are formatted in a standard fashion, the tool will export all active points to a PDB file. So turn off anything you don't want in your PDB. Also, if it encounters an non-standard atom name, it will output "UNK" in the atom field of the PDB.

Chapter 3

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.

3.1 Exporting for POV-Ray

KiNG can produce output script files to be fed into the high-quality free raytracing program POV-Ray (www.povray.org). POV-Ray can generate all kinds of "photo-realistic" effects including different materials and lighting schemes, simulated depth of field, *etc.* It is also very useful for producing digital movies that may be more convenient to use during talks and presentations. (I recommend the inexpensive QuickTime Pro from Apple for stitching together all the output images into a movie.) The POV file is largely complete as written and includes terse hints for rendering, but if you use this feature much you'll probably want to learn something about POV-Ray and tweak the scripts before rendering them. Most of the things you'll want to change are either at the very top (colors, textures, and sizes of things) or at the very bottom (camera viewpoint, depth cueing, lighting).

3.2 Deprecated export formats

These feature now lag far behind the rest of the program in functionality; they may not work at all. For this reason, they do not appear in the menus by default and must be "enabled" under the Tools menu. If you need any of these capabilities, 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 ;)

KiNG also 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 4

Copyright & acknowledgments

4.1 Copyright

4.2 Revision status

This manual was last updated 30 May 2005 by VBC for Extratools version 1.00 (added chapter about kinemage editing).