The Chiropraxis tools manual

Ian W. Davis

1st April 2005

Chapter 1

The Tools

1.1 BACKRUB Tool: Protein chiropraxis

The BACKRUB tool is used to adjust short segments of protein backbone without disturbing the surrounding structure. It allows you select one residue, and rotate it around the axis between its neighboring C-alphas. Using BACKRUB requires that `chiropraxis.jar` be present in the `plugins/` folder.

Create a backrub by control-clicking the alpha carbon of the central residue. 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 BACKRUB 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.

BACKRUB has not been published as of 1 April 2005. When it is, a citation will appear here.

1.1.1 Command reference

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

1.2 C-alpha Hinges

Hinges is the generalized version of BACKRUB. It allows you to select any continuous region of backbone that joins two alpha carbons, and then rotate that segment of backbone around an axis drawn between those C-alphas. Individual peptides can also be rotated. Create a hinge by control-clicking the two alpha carbons that act as its endpoints or anchors.

Regions longer than two peptides (*i.e.*, what BACKRUB handles) are seldom useful in fitting structures. Thus, this tool has been largely superceded by BACKRUB.

1.3 Sidechain Rotator: Refitting protein models

The Sidchain 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 rotamericity 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.

1.4 Sidechain Mutator: Redesigning protein models

The Sidchain 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.

1.5 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.

Chapter 2

Copyright & acknowledgments

2.1 Copyright

2.2 Revision status

This manual was last updated 1 April 2005 by IWD for Chiropraxis version 0.45.