

The Chiropraxis tools manual

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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 is described in the following publication: I.W. Davis, W.B. Arendall III, D.C. Richardson, and J.S. Richardson (2006) "The backrub motion: How protein backbone shrugs when a sidechain dances" Structure 14, 265-274.

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 superseded by BACKRUB.

1.3 Shear Tool: Helical winding plus unwinding

The shear tool can be used to modify backbone, most commonly helix, in a manner almost completely orthogonal to the backrub. A shear shifts three peptides instead of two like a backrub, and moves the central peptide nearly parallel to the chain direction rather than perpendicular to it. Use Ctrl+Click (a.k.a. middle-click) to select a residue; it, its preceding residue, and its two following residues will become the active “molten” state. Next, drag the primary shear dial for the main motion, then optionally drag the three peptide rotation dials to alleviate some strain. Functionality is generally similar to the backrub tool.

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1.4 Tweak Phi/Psi: Visualizing possible backbone changes

The tweak phi/psi tool is useful for slightly altering the backbone dihedrals phi and psi. Use Ctrl+Click (a.k.a. middle-click) to select a residue and its adjacent region as the active “molten” state. The length of the active region can be customized by entering a number of residues in the box and pressing enter. Next, drag the phi/psi dials to rotate the molten region around either the phi or psi axis. Note that this tool

makes no attempt to close the resulting chain break or to alleviate the steric clashes it usually introduces, and thus should not be employed as a fitting tool. However, it can be useful for visualizing the local effects of small changes in ϕ/ψ and simply building intuition.

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1.5 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.

1.6 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.

1.7 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:

- Backrub
- C-alpha hinges
- Shear

- Tweak phi/psi
- 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

The Chiropraxis code and all its associated original resources and documentation are copyright (C) 2002-2010 by Ian W. Davis, Daniel A. Keedy, and Vincent B. Chen.

2.2 Revision status

This manual was last updated 1 September 2010 by DAK for Chiropraxis version 1.07.