

Swiss PDB Quick Card for Apple - from Jake Jaffee

Translate view Rotate View Measure Angle Identify atom Choose center of rotation Change an AA

Center visible (same as =) Zoom View Measure distance Display relevant angles for an atom Select proximal groups Manually align two layers Change local torsion angles

global/local coordinates Display PDB file Move all / selection toggle info window (sometimes)

Help Perspective indicator

Web resources:

SwissPDB Website: <http://expasy.cbr.nrc.ca/spdbv/>
- contains user guide and tutorial

The PDB: <http://www.rcsb.org/>
- where you can obtain structures (PDB files)

VERY USEFUL:

"=" key to center on visible groups
"enter" key (on numeric keypad) to toggle "show" column for selected groups

Control Panel: Status

Group visible? Sidechain visible? Toggle labels Surface Visible? Ribbon Visible?

Toggle layer visibility Chain code 2' structure type Amino acid/position

group	show	side	label	rib	col	BS
4 THR10	✓	✓	✓	✓		
4 s ALA11	✓	✓	✓	✓		
4 s THR12	✓	✓	✓	✓		
4 s LEU13	✓	✓	✓	✓		
4 s CYS14	✓	✓	✓	✓		
4 s LEU15	✓	✓	✓	✓		

Surface type selector:
 VDW(v)
 Accessible(a)
 Molecular(m)
 User(u)

Color apply selector and indicator:
 Backbone + sidechain (BS)
 Backbone (B)
 Sidechain (S)
 Ribbon (R)
 Label (L)
 Surface (U)

Selection Status:
 RED = selected
 BLACK = unselected

Rotation Constraints:
 Control = X Axis
 Option = Y Axis
 Apple = Z Axis

Control Panel: Actions

Click column header to limit to selected only Click to change color for all selected AA

group	show	side	label	rib	col	BS
4 THR10	✓	✓	✓	✓		
4 s ALA11	✓	✓	✓	✓		
4 s THR12	✓	✓	✓	✓		
4 s LEU13	✓	✓	✓	✓		
4 s CYS14	✓	✓	✓	✓		
4 s LEU15	✓	✓	✓	✓		

Click to select chain Click to select 2' structure element Click to select A.A.

Click to toggle in these columns. Shift-click to toggle all for the column.

Click to change color of one AA

Selection modifiers:
 Control-click = add to current selection (this works for menu selections, too!)
 Shift-click = select range of AA

Notes:
 The show column must have a for sidechain, label, or surface to be shown. The ribbon column is independent of this.

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Legend: z = apple key = shift key

File menu:

z O Open PDB file
z W Close current layer
z W Close all layers (buggy)
z S Save layer
z S Save project (all layers + orientation)
z E Save image
z E Save stereo image

Edit menu:

z Z Undo
z Z Redo
z X Cut
z C Copy
z V Paste
z F Find sequence
z F Find next instance

Select menu:

z 0 Select none
z A Select all
z 1 Invert selection
z P Pick on screen (Esc to stop)

Fit menu:

z M Magic fit two structures
z M Best fit two structures
z D Calculate RMSD
z G Generate structural alignment

Display menu:

z 2 Bottom perspective
z 4 Left perspective
z 5 Front perspective
z 6 Right perspective
z 7 Back perspective
z 8 Top perspective

z / Slab
z T Stereo
z H Show hydrogens (if present)
z B Show H-bonds (must calculate first!)
z 3 3-D mode

Labels:

z U Group name
z J Atom name
z K Atom type
z - Clear user labels (distances, etc.)

Windows:

z ' Toolbar
z , Control Panel
z L Alignment (seq)
z I Layer info
-
z R Ramachandran plot
z I Electron Density map (if loaded)
z \$ Text window (if in background)

Note: Items in the Color menu apply to all groups, not just selected groups.

Common actions:

Focus in on a couple of amino acids (or groups):

1. Select the amino acids of interest by clicking on their code in the Control Panel (ex: LYS84). They will turn red. Hold the Control or z key to select multiple amino acids.
2. Click on the "show" column header in the Control Panel. This will limit the display to selected groups.
3. Press the "=" key. Your selection will be zoomed.
4. (Optional) Click on the "labl" column header. The amino acids will be labeled.

Make a Branden & Tooze style cartoon diagram:

1. Select all (z A)
2. Click "ribn" in Control Panel
3. Shift-click on a in the "show" column.
4. Click and hold the downward arrow under "col" until a menu appears. Choose "ribbons."
5. In the Color menu, choose "Secondary Structure Succession"
6. (optional) In the Display menu, choose "Render in solid 3D" Make sure that "Render as solid ribbon" is checked in the Ribbons... item of the Prefs menu.

Show Hydrogen Bonds:

1. Select and display the part of the structure for which you want to see the H-bonds. Only groups that have the "Show" item checked in the control panel will display H-bonds.
2. In the Tools menu, choose "Compute H-bonds".
3. If H-bonds do not appear, press z B (Show H-bonds)

Display the surface of a structure:

1. Select all (z A)
2. In the Tools menu, choose "Compute Molecular Surface".
3. (Optional) In the Display menu, choose "Render in solid 3D".
4. To get rid of the surface, from tile File menu, choose Discard... and then the Surface option.

See a slice through a structure (slabbing):

1. Press z /.
2. To change the position of the slice, hold the Shift key while moving the mouse up and down.
3. To change the width of the slice, from the the Prefs menu, choose Display... and edit the Slab Depth parameter. The default is 10 A.
4. Press z / again to end slabbing.

Quickly superimpose two similar structures:

1. Load both structures into the SwissPDB-Viewer. They will appear on separate layers.
2. Press z M. A dialog box will appear. Click "OK".

See just the backbone of a structure:

1. Select all (z A).
2. Click the "show" column header in the Control Panel.
3. Shift-click on a in the "side" column.