

PYMOL TRICKS

A COMPILATION OF RECIPES

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Installing pymol nowadays is very easy in almost any Linux version with a package management system like yum or apt-get. For more information on this the pymolwiki at <http://pymolwiki.org> is the best resource. The following is just a compilation of tricks for pymol power-users.

- GENERAL

```
bg white # Turn background color to white
save rna6.pse # Save your working session to pse file
set valence, 1 # Show double bonds.
h_add # Show hydrogens.
pymol -qc bla.pml >& bla.log & # To invoke without X11 display
pymol -M # Invoke mono mode instead of stereo
# to avoid flicker in some screens.
unbond (id 8), (id 2) # Remove a bond between atoms
bond (id 8), (id 2) # Create a bond between atoms
select carbons, symbol c # Select all carbon atoms and call them carbons.
color black, carbons # Color the carbons selection black.
disable selectionname # Hides/disables a loaded structure(selection).
enable selectionname # Shows/enables a loaded structure(selection).
set internal_gui, 0 # Hide object control panel
```

- LABELS

```
label (n;Cl'), "%s" % (name)
set label_color, black
set label_font_id, 4
set label_size, 3
set label_position, [2,0,0]
show labels
```

- SPHERES

```
set sphere_scale, 0.25
```

- STICKS

```
show sticks, selectionname
set stick_radius, 0.1
set stick_ball, on #Makes the stick command show ball and stick
set stick_ball_ratio, 1.5
```

- RIBBONS

```
set ribbon_color, marine
set ribbon_width, 2
set ribbon_sampling, 1
set ribbon_smooth, 1
```

- CARTOON

```
cartoon putty
set cartoon_ladder_mode, 0
set cartoon_transparency, 0.5
set cartoon_ring_finder, 0
cartoon dumbbell
set cartoon_dumbbell_width, 0.2
set cartoon_dumbbell_radius, 0.4
set cartoon_color, marine, resi 34-67
set cartoon_color, blue, resi 68,78
show cartoon
```

- RAY TRACING

```
set ray_trace_mode, 3
set ray_trace_fog, 0
set ray_shadows, 0
set depth_cue, 0 #This one with care or it might look funky.
set antialias, 1
set ray_trace_gain, 0.005
ray 1600,1200
png img1.png
```

- ROTATING

"turn" to rotate all loaded objects, "rotate" for individual objects

```
turn x, 10
```

Definition of Objects and Selections found at:

http://pymolwiki.org/index.php/Objects_and_Selections

- IMPORTANT SETTINGS

orthoscopic (0 or 1) controls whether the OpenGL renderer uses the same orthoscopic transformation as the renderer. You'll want to set this to 1 when preparing figures so that OpenGL and raytracing match pixel-for-pixel.

ambient (0.0-1.0) controls the ambient light intensity for both OpenGL and the ray-tracer.

ambient_scale (float) controls the relative ambient intensity between OpenGL and the ray-tracer.

antialias (0 or 1) generate a "smooth" image (best quality, but takes 4X as long).

direct (0.0-1.0) the planer light intensity originating from the camera.

gamma (0.1-2.0) gamma transformation applied after rendering is complete.

light (vector) the position of the light.

reflect (0.0-1.0) the planer light intensity originating from the light source.

spec_reflect (0.0-1.0) intensity of the specular reflection from the light.

spec_power (1-100) how localized is the specular reflection (higher=smaller).

ELECTROSTATIC POTENTIAL MAPS

Go to: http://nbc-222.ucsd.edu/pdb2pqr_1.8/

Upload your pdb or use one id you like.

Download the resulting pqr file

open in pymol

```
color white
color blue, (pc; > 0.1)
color red, (pc; < 0.1)
show surface
```

RAY TRACING

To ray trace an image with an opaque background.

```
# turn on transparent alpha channel
set ray_opaque_background, off
```

GENERAL TIPS

Shift-right_click and slide controls fog intensity and after a point it starts clipping.

Shift-wheel controls fog intensity and after a point it starts clipping.