Pymol Reference Card

Modes
Pymol supports two modes of input: point and click mode, and command line mode. The point and click mode allows you to quickly rotate the molecule(s) zoom in and out and change the clipping planes. The command line mode where commands are entered into the external GUI window supports all of the commands in the point and click mode, but is more flexible and possibly useful for complex selection and command issuing. Commands on the command line are executed when you press the return key.

Basic Commands
Some commands used with atoms selections. If you are unsure about the selection, click on the molecular or part that you want in the viewing window and then look at the output line to see the selection.

Loading Files
file loading load data/test/pept.pdb
loading from terminal pymol data/test/pept.pdb
toggle between text and graphics Esc

Mouse Control
Atom Selection
object-name/segi-id/chain-id/resi-id/name-id
molecular system selection /pept
molecule selection /pept/lig
chain selection /pept/lig/a
residue selection /pept/lig/a/10
atom lig/a/10/12/2a
ranges lig/a/10-12/2a
rules a+6+8+c0
missing selections /pept/a

Cartoon Settings
Setting the value at the end to 0 forces the secondary structure to go through the CA position.
cylindrical helices set cartoon.cylindrical.helices,1
fancy helices [tubular edge]
cartoon_fancy.helices,1
flat sheets cartoon.flat.sheets,1
smooth loops cartoon.smooth.loops,1
find rings for cartoon cartoon.ring_finder,[1,2,3,4]
set ring mode cartoon.ring_mode,[1,2,3]
nucleic acid mode set nucleic.acid_mode,[0,1,2,3,4]
cartoon sidechains set cartoon.side_chain_helper;
rebuild primary colour set cartoon.color.blue
secondary colour set cartoon.highlight_color.grey
set cartoon_discrete_colors,on
set cartoon_transparency,0.5
cartoon loop cartoon_loop
cartoon loop cartoon_loop_rectangular
cartoon oval cartoon_oval
cartoon tubular cartoon_tubular
cartoon arrow cartoon_arrow
cartoon dumbell cartoon_dumbell
b-factor sausage cartoon.putty.a

Cartoon Transparency
set cartoon_transparency,0.5

Image Output
low resolution
high resolution
ultra-high resolution
change the default size [pts]
image shadow control
image fog control
image depth cue control
image antialiasing control
export image as .png

Hydrogen Bonding
Draw bonds between atoms and label the residues that are involved.
draw a line between atoms /pept
set the line dash gap set dash_gap,0.09
set the line dash width set dash_width,3.0
set the line dash radius set dash_radius,0.0
set the line dash length set dash_length,0.15
set round dash ends set dash_round_ends,on
hide a label label, dist01
label a residue label (542/oe1), "%s %("E542")
set label font set label_font,4
set label colour set label_color,white

Electrostatics
There are a number of ways to apply electrostatics in Pymol. The user can use GRASP to generate a map and then import it. Alternatively the user can use the APBS Pymol plugin. Pymol also has a built in function that is quick and dirty.
generate electrostatic surface action > generate>vacuum
electrostatics > protein contact potential

Pymol Movies (mac)
move the camera move x,10
turn the camera turn x,90
play the movie mplay
stop the movie stop_movie
writeout png files mpng prefix [, first [ , last] ]
show a particular frame frame number
move forward on frame move_back one frame
go to the start of the movie backwards
go to the middle of the movie forward
go to the movie end end
edit the current frame get_frame
execute a command in a frame mdo 1, turn x,5; turn y,5;
dump current movie commands mdump
reset the number of frames per second meter_reset
Miscellaneous
add hydrogens in to a molecule selection
alias a set of commands separated by ";" 
1hpv.pdb; zoom 200/; show sticks, 200/ around 8
structurally align
object=alignment
fit one molecule to another
create a new selection
delete a selection
save file
create a new selection
delete selection
add alias a set of commands separated by ";"
alias go,load
1hpv.pdb; zoom 200/; show sticks, 200/ around 8
structurally align
align prot1///CA, prot2,
object=alignment
fit one molecule to another
copy at selection
create target, selection
delete selection
save file
protect or deprotect a selection
set color name, rgb

Secondary Structures
Pymol has a secondary structure determination algorithm called dss, however it is better to use the DSSP algorithm and then define the limits manually.
to run dss
to define helical structure
alter 11-40/, ss='H'
to define loop regions
alter 40-50/, ss='L'
to define strand structure
alter 50-60/, ss='S'
rebuild the cartoon after alteration
get dihedral angle
get_dihedral 4/n,4/c,4/ca,4/cb

Files
change the working directory
change cwd to <path>
lst contents of current directory
ls
print current working directory
pwd

Crystal Structures
To recreate crystal packing of molecules within 5 Å of pept in the pept.pdb (which must contain CRYST date), use the sympol command. 
sym,pept,(pept),5.0

NMR Structures
NMR models should be loaded into the same object, but should have different states. load a model into an object
load file.pdb, object
show all models in an object
set all_states,1
show only one object model
set all_states,0
show a particular model
frame model_number
get_model
fit two structures to one another
fit selection
fit and calculate the rms
rms selection
rms without fitting
rms_cur selection
fit ensemble structures
intra_fit selection,1
enqueue rms
intra_rms selection,state
ensemble rms without fitting
intra_rms_cur selection
set the current model
set_all_states,1

Changing Structures
add a bond
bond atom1, atom2
remove bonds
unbond atom1, atom2
join to molecules together
fuse [atom1, atom2]

Old School Images
Load a .pdb and make a cartoon view. Then change the background colour to white and change the ray mode to 2.
set ray_trace_mode,2
make the lines thinner
set antialias,2
raytrace the image
ray