Common commands in three molecular visualization programs

action	Rasmol	Chimera	Pymol
simplified display for overview	*Display->Cartoon* *Colours->Chain*	*Actions->Ribbons->Show* *Actions->Atoms/Bonds->Hide* *Tools->Depiction->Rainbow->Chain*	*all->H->Hide everything* *all->S->Show cartoon* *all->C->Color by chain->by chain(e. c)*
identify an atom in the display	*click on atom* *e.g:Atom: CD2 1633 Group: HIS 77 Chain: B Model: 1*	*hover the cursor over the atom* *e.g:#0.1 LYS 66.B CG* *ctrl-click to select (ctrl-click backgrnd to deselect)*	*click selects residue and prints:* */file/model/group/chain/residue/atom* *e.g.: /2dn1//B/HIS`92/NE2*
zoom in	*shift-click*	*right-click*	*right-click*
adjust clipping planes	ctrl-leftclick	*Favorites->Side View*	shift-rightclick
select key residues	**`RasMol> select his87`**	**`command> select #0:87.A`**	**`PyMol> select His87, HIS`87/`**
display heme as sticks	**`RasMol> select HEM`** *Display->Sticks*	*Select->Residue->HEM* *Actions->Atoms/Bonds->Show* *Actions->Atoms/Bonds->Stick*	**`PyMol> select hemes, resn HEM`** *(hemes)->S->Show sticks* *(hemes)->C->Show sticks*
export nice picture	N/A	*Tools->Viewing->Effects->Subdivision Qual.>5* *File->Save Image->Save As*	**`viewport 2000,1500`** increases resolution **`ray`** creates ray-traced image **`png`** saves it as .png file
define a group to work with	**`RasMol> define keyHis, his87`**	*Select->Name Selection*	**`PyMol> select His87, resn his`**
structural alignment	N/A	*Tools->Structure Comaparison->MatchMaker*	**`PyMol> align prot1////ca,prot2`**
calculate missing secondary structure	**`RasMol> structure`**	**`command> ksdssp`** `selection`	**`PyMol> dss`** `selection`
display electrostatic surface	**`N/A`**	calculate using GRASP (another program) *Tools->Surface/Binding Analysis->Electrostatic Surface Coloring*	*(1ubi)->A(ctions)->generate->vacuum electrostatics->protein contact potential (local)* [or *Plugin->APBS tools*]
example script	pdb_compare.rasmol	pymol_complex_compare.pml	pymol_complex.pml
online user manual	http://www.umass.edu/microbio/rasmol/distrib/rasman.htm	http://www.cgl.ucsf.edu/chimera/docs/UsersGuide/index.html	http://pymol.sourceforge.net/newman/user/toc.html