

Help for a given command **help command_name**

Loading structures

Load from hard disk **load /path/filename.pdb** (optional: , name)
 Retrieve from PDB **fetch 1UBQ** (or any other PDB ID)

Navigating

Orient (centers view): **orient 1UBQ** (or another selection)
 Reset view to cover everything: **reset**

Selection

All selections can be combined with “and”, “or”, “not” logic. Parentheses give hierarchy.

Basic selection pattern: **select name, what_to_select**

molecule name **1UBQ** (name as listed in the names panel)

residues by number **resid 10,51**

residue range **resid 10-70,80-90**

residues by type **resn lys**

chain **chain A**

atom name **name ca**

element **elem O**

secondary structure **ss S** (S selects strands; H helices; “” loops)

example: **select helix, 1UBQ and (resid 10-60) and name ca and ss H**
 selects the α -carbons (name ca) of all residues that fall between residues 10 and 60 and are part of an α -helix.

complex example: **select link, 2JF5 and ((resid 68) and chain A and not (name c+o+n)) or ((resid 76) and chain B and not (name n))**
 selects the side chain of residue 68 in chain A and everything but the amino group of residue 76 in chain B.

Change name of selection: **set_name old_name, new_name**

Changing representations

Show: **show cartoon, 1UBQ and ss H**

Hide: **hide sticks, 1UBQ and (resid 48,63)**
cartoon, ribbon, sticks, lines, surface, spheres, nonbonded, everything (and more)

Coloring

Background color: **bg_color white**

Basic coloring: **color yellow, (resid 40-60) and elem C**

Color a certain representation: **set cartoon_color, yellow, 1UBQ and ss H**

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