1a

load molecule

By PDB code: [____] [load] [append]
- ● Asymmetric Unit ○ Biological Assembly

From Proteopedia uploaded file:
[____] [load] [append]

(To load from an uploaded file, first upload the file to Proteopedia)

☐ Add both hydrogens and multiple bonding while loading the structure.

2

build your selection

groups:
- all
- *protein*
- all protein
- alpha carbon
- backbone/mainchain
- helix
- sheet
- sidechain
- turn
- *non-protein*

Hold ctrl to select multiple groups

sites:
- all atoms

limit to chains:
all
e.g. A,C,D

limit to residue types:
all
e.g. PHE,ALA,GLY

limit to residue numbers:
all
e.g. 18,23-25,32

limit to elements:
all
e.g. Fe,2H,31P

[replace selection] [add to selection]
[remove from selection]

invert and center

[invert current selection] [center on current selection]

select within distance

Select atoms within [____] Å of current selection. [go]
Expand selection to include entire residues containing any selected atoms. [go]

mouse click selects

○ nothing ○ center ○ atom ○ element ○ residue/ligand ○ chain

3a

set selection representation

☐ ball and stick ☐ stick/wireframe 90
☐ spacefill 100% ☐ dots 100% ☐ backbone 90
☐ trace 90 ☐ ribbon ☐ cartoon
☐ strands ☐ rocket ☐ meshribbon 2.5
☐ surface ☐ halos ☐ slab / depth 100 0

Leaving the input field to the right of a representation-type blank chooses its default setting.
Ball and stick is a combination of wireframe and spacefill.

[replace representation] [add to representation]
[remove from representation]
[hide selection]

disulfide and hydrogen bonds [hide]

ssbonds on (backbone) ▾ color ▾
hbonds off ▾ color ▾

3b

color

● selection ○ background ○ isosurface ○
caption_Background_Color ○ caption_Font_Color [Demo Caption]

[color palette grid]

[elements (CPK)]   [chain]
[composition]
[N->C rainbow (named chain)] [N->C rainbow (polymer)]
[secondary structure]   [hydrophobic/polar]
[charge, protein]   [evolutionary conservation]
[temperature, fixed]   [temperature, relative]

transparency

[0] % transparent [go]

3c

mouse click selects

● nothing ○ atom

label selected atoms

text: [____]

☐ atom name ☐ element ☐ 3-letter residue code
☐ residue # ☐ chain
[set label] [clear labels from selection]
labels are set to each atom in a selection

color ▾ label size... ▾ font... ▾
pointer off ▾

Label position: x offset [4] y offset [4]

caption [show]

measurements [show]

4

Check for
- centering
- spare parts
- in frame
- occlusions
- orientation

5

Save current scene

Scene name
[____]

e.g. Active_site_gorge
Enter an existing scene name to save as the most recent version (will not overwrite).

Scene description, for your own record
[____]

Scene caption for display under JSmol applet
[____]

when this scene loads, I want it to [stay still ▾]
[Use Default Rendering While Rotating ▾]

☐ Always Reload Structure When Loading this Scene

show scene transition options? ☐

[Save current scene]

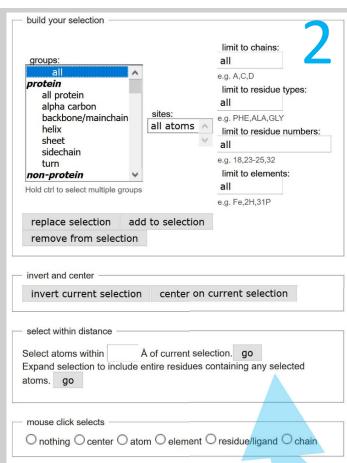## 1b

load scene

Page name
[User:Karsten_Theis/BioMolViz]
A Proteopedia page name.

Scene name   Version number
[Choose... ▾]   [▾]

SAT workflow

1: load molecule or scene
2: select atoms
3: draw, color, label
4: check scene
5: save scene
6: insert green link

6

Scene Link
Scroll-up to the the main edit area of the page, and position the cursor at the place where you would like the green link to appear. Otherwise select, within the main edit area of the page, a portion of text that will become the green link. After that, click on the button to [Insert Scene Link]