1a — load molecule

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.

1b — load scene

load scene

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

Scene name
Choose...

Version number
[ ]

2 — build your selection

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

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

color

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

elements (CPK)
composition
N->C rainbow (named chain)
secondary structure
charge, protein
temperature, fixed

chain
N->C rainbow (polymer)
hydrophobic/polar
evolutionary conservation
temperature, relative

transparency
0 % transparent go

3c — mouse click selects

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

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

6 — Scene Link

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

SAT workflow

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

Available under Jmol window

Select Atoms ○ ALL ○ NONE
Show Selected with Halos ○ ON ○ OFF
<-Undo Redo->
Use Simplified Rendering While Moving ⌄
Advanced: Open JSmol Console
or enter below JSmol commands
help
Execute

Reference:
search
scene authoring tools
Go   Search

proteopedia.org/w/Scene_authoring_tools