# SAT workflow

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

## 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

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]

## 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.

## 1b — load scene

Page name
User:Karsten_Theis/BioMolViz
A Proteopedia page name.
Scene name          Version number
Choose... ∨          ∨

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

Available under Jmol window

## 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

## 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

## Reference:

search
scene authoring tools
Go   Search

proteopedia.org/w/Scene_authoring_tools