SAT (Scene Authoring Tools)

SAT workflow
1: load molecule or scene
2: select atoms
3: draw, color, label
   repeat 2+3 as needed
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
Nucleic acid

Hold ctrl to select multiple groups

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

sites:
all atoms
HEM-OXY

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

limit to residue numbers:
all
e.g. 18,23-25,31

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

replace selection | add to selection | remove from selection
limit 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

clear Selections Tab

2b

Select Atoms ● ALL ○ NONE (1 atoms currently selected)
Show Selected with Halos ○ ON ● OFF
<-Undo | Redo->
Use Simplified Rendering While Moving
Advanced: Open JSmol Console
or enter below JSmol commands - Useful one-liners
help | Execute

3a

set selection representation

☐ ball and stick ☑ stick/wireframe 60 ☐ spacefill 100%
☐ dots 100% ☐ backbone 90 ☐ trace 90 ☐ ribbon
☐ cartoon ☐ strands ☐ rocket
☐ meshribbon 2.5 ☐ surface ☐ halos

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

replace representation | add to representation
remove from representation

center on current selection | center on visible atoms
hide selection ☐ zshade ☐ slab / depth 100 0

disulfide and hydrogen bonds [hide]
ssbonds on (backbone) | color
hbonds off | color

clear Representations Tab

4
Check for
• centering
• spare parts
• in frame
• occlusions
• orientation

5

Save current scene
Scene name
Detail
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
The iron atom (orange) is complexed by six atoms (four nitrogen atoms from the porphyrin ring, one nitrogen from His 93, and one oxygen atom from the bound dioxygen, red spacefill).

when this scene loads, I want it to spin on Y axis
Use Default Rendering While Rotating

☑ Always Reload Structure When Loading this Scene
show scene transition options? ☑

scene transition options
skip the zoom-out when this scene loads? yes
skip the transition between scenes when this scene loads? yes

Save current scene

1a

load scene
Page name
Karsten_Theis/myoglobin
A Proteopedia page name.
Scene name | Version number
Detail | 10
Scene description

Scene caption
The iron atom (orange) is complexed by six atoms (four nitrogen atoms from the porphyrin ring, one nitrogen from His 93, and one oxygen atom from the bound dioxygen, red spacefill).

WikiText
Copy and paste the following line where you want the scene link to appear (scroll down if needed):
<scene name='86/865266/Detail/10'>TextToBeDisplayed</scene>
Upon loading a scene, wikitext for creating a link to the loaded scene will appear above.

1b

load molecule
By PDB code: [ ] load
● Asymmetric Unit ○ Biological Assembly
From Proteopedia uploaded file: [ ] load
(To load from an uploaded file, first upload the file to Proteopedia)
☑ Add both hydrogens and multiple bonding while loading the structure.

how to
1a load scene
1b load molecule
2 selections
→ **2b**
3a representations
3b colors
3c labels
5 save scene
Reset SAT

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

measurements [hide]
color | size... | units... | labels on
delete all measurements

3b

color
● selection ○ background ○ isosurface
caption_Background_Color | caption_Font_Color | Demo Caption

elements (CPK) | composition | chain
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

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
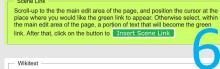
Wikitext
Copy and paste the following line where you want the scene link to appear (scroll down if needed) and edit the TextToBeDisplayed:
<scene name='86/865266/Detail/16'>TextToBeDisplayed</scene>
Upon saving a scene, wikitext for creating a link to the saved scene will appear above.