

The following shows JmolShell commands that can be embedded in your HTML file:

Link within text

Your reader can click on links in the text, for example to [show arginines in light blue](#)

```
<script>jmolLink("select Arg;color lightblue;wireframe 80", "show arginines in light blue")</script>
```

Script to be run when link is clicked

Text that should be the link

Toggle Checkbox

You can also set up toggle boxes:
☐ Protein red

Text that should be displayed next to the check box

```
<script>jmolCheckbox("select protein;color red","select protein;color cpk","Protein red","")</script>
```

Script to be run when toggle is turned "on"

Script to be run when toggle is turned "off" - should "undo" first set of commands

Toggle a Monitor Line between Two Atoms

☐ Distance between atoms 331 & 1381

Text that should be displayed next to the check box

```
<script>ToggleMonitor(331,1381,"Distance between atoms 331 & 1381")</script>
```

AtomNo for first atom

[ALA]41:P.CA #331

AtomNo for second atom

[C]7:D.O2 #1381

Two show 2 separate distances at once, use jmolCheckbox and include the scripts yourself.

The following shows the sections of a presentation with 3 user menus. The actual content is in the file "index.html." This is the file that you load into a browser.

Page 1 (this page) is required, and is the basic setup page. Here you tell the program where to find your pdb file (should be in the same folder), a "reset," or setup script, and provide information on the source of the data (PDB id, literature citation). Finally, you include your name and the date your file was most recently updated.

Setup Section - Change text in circles, but ONLY the text in circles!

```
<!DOCTYPE HTML PUBLIC "-//W3C//DTD HTML 4.01 Transitional//EN"
    "http://www.w3.org/TR/html4/loose.dtd" >
<HTML><HEAD>

<!-- The following loads the Jmol package of scripts -->
<script src="../../Support/Jmol.js"
        LANGUAGE="JavaScript1.2" type="text/javascript"></script>
<noscript>
This site requires that JavaScript (and JAVA) be enabled in your browser.
</noscript>

<SCRIPT LANGUAGE="JavaScript1.2" type="text/javascript" src="../../Support/JmolShell.js">
</SCRIPT>

</HEAD><BODY BGCOLOR="#FFFFFF">

<script>
    JmolAppl(
        "struct.pdb",      // the name of the pdb coordinate file
                          // change this to point to your pdb file
        "Reset.txt",      // file containing an initializing script
                          // point to a file containing a script to
                          // initialize the view
        "1DP7",           // PDB code for the structure
                          // for the users' edification
                          // and for proper auto-citation
                          // a description of the structure
                          // (again, for the users' edification)
        "Winged Helix-Protein Hrfx1 with its X-box binding site",
                          // citation for the structure
        "K. S. Gajiwala et al., Nature 403, 916 (2000)",
        "10706293",       // Pubmed id number
        "Craig Martin",   // Author of this presentation (your name)
        "October 10, 2004", // Date this presentation was last updated
        "../../Support/"  // path to the support folder
                          // must point to the folder containing the files
                          // jScripts.txt, empty.html, jMenu.html et al
                          // the Jmol folder must also be here...
    );
</script>
```

User menu page I - put your code here

```
<SCRIPT> StartNewDiv( "Basics" , "Introduction" )</SCRIPT>
```

This signals the beginning of a new section

<H3>**Just the basics**</H3>

Your reader can click on links in the text, for example to `<script>jmolLink("select Arg;color lightblue;wireframe 80", "show arginines in light blue")</script>`

<P>

You can also set up toggle boxes:

```
<BR><script> jmolCheckbox( "select protein;color red", "select protein;color cpk",  
                          "Protein red", "" )</script>
```

```
<BR><script> jmolCheckbox( "select nucleic;color green", "select nucleic;color cpk",  
                          "DNA green", "" )</script>
```

<P>

```
<script> ToggleMonitor(331,1381, "Distance between atoms 331 & 1381")</script>
```

User menu page II - put your code here

```
<SCRIPT> StartNewDiv( "Intro" , "Introduction" )</SCRIPT>
```

This signals the beginning of a new section

This is an example of a **Jmol presentation** (click on the "About" menu above for more info on Jmol).

<HR>

The protein is the winged-helix DNA-binding protein Hrfx1, bound to its X-box binding site

<P>

This is a classic example of direct read-out via the `<script>jmolLink("select DNA;wireframe off;cartoon off;backbone off;spacefill 500", "major groove")</script>` .

<P>

One can see some of the major groove `<script>jmolLink("select all;cartoon off;spacefill off;wireframe off;backbone off;select protein;backbone 120;select nucleic;wireframe 80;select protein and (19 or 39 or 41 or 45 or 48 or 66 or 67 or 69 or 58 or 57 or 60);wireframe 100;select nucleic and within(3.5,protein);spacefill 140;color cpk;select protein and within(3.5,nucleic);spacefill 140;color cpk", "protein-DNA contacts")</script>`

and can actually show some `<script>jmolLink("monitors off;monitor 474 1668;monitor 364 1362;monitor 364 1355;monitor 475 1462;monitor 474 1465;monitor 364 1355;monitor 364 1355;monitor 461 1633;monitor 464 1621;monitor 390 1389;monitor 388 1388", "reasonable distances")</script>` for H-bonding and electrostatic interactions.

<HR>

Show me the protein `<script>jmolLink("select protein and hydrophobic and not surface;spacefill 400", "hydrophobic core")</script>` .

<P>

Show me the protein `<script>jmolLink("select protein and buried;spacefill 400;color gray;select protein and surface;spacefill 400;color pink", "hydrophobic core")</script>` a different way.

<P>

Show me the hydrophobic core, yet another way:


```
<BR><script> jmolCheckbox( "select protein and buried;spacefill 400;color gray",  
                        "select protein and buried;spacefill off;color cpk", "Buried", "" )</script>
```

```
<BR><script> jmolCheckbox( "select protein and surface;spacefill 400;color pink",  
                        "select protein and surface;spacefill off;color cpk", "Surface", "" )</script>
```

User menu page III - put your code here

```
<SCRIPT> StartNewDiv( "More details" , "fancier stuff here") </SCRIPT>
```

This signals the beginning of a new section

Often, it is easier to turn specific interactions on and off using "checkboxes"

```
<P>
```

```
<H3>Protein-DNA contacts</H3>
```

```
<script> jmolCheckbox( "select protein and 58;wireframe 95","select protein and 58;wireframe  
off" , "Toggle Arg58" , "off" )</script>
```

```
<script> jmolCheckbox( "select all;cartoon off;spacefill off;wireframe off;backbone off;select  
protein;backbone 120;select nucleic;wireframe 80;select protein and 58;wireframe 100;monitor  
474 1465;monitor 475 1462;select atomno=474 or atomno=475 or atomno=1462 or atomno=  
1465;spacefill 140" ,"monitor 474 1465;monitor 475 1462;select atomno=474 or atomno=475 or  
atomno=1462 or atomno=1465;spacefill off" ,"Arg58 to G11" , "" )</script>
```

```
<BR>
```

```
<script> jmolCheckbox( "select all;cartoon off;spacefill off;wireframe off;backbone off;select  
protein;backbone 120;select nucleic;wireframe 80;select protein and 45;wireframe 100;monitor  
364 1362;monitor 364 1355;select atomno=364 or atomno=1362 or atomno=1355;spacefill  
140" ,"monitor 364 1362;monitor 364 1355;select atomno=364 or atomno=1362 or atomno=  
1355;spacefill off;select protein and 45;wireframe off" ,"Lys45 to C6 phosphate & sugar" , "" )</  
script>  
<BR>
```

```
<script> jmolCheckbox( "select all;cartoon off;spacefill off;wireframe off;backbone off;select  
protein;backbone 120;select nucleic;wireframe 80;select 57 and protein;wireframe 100;monitor  
461 1633;monitor 464 1621;select atomno=461 or atomno=1633 or atomno=464 or atomno=  
1621;spacefill 140" ,"monitor 461 1633;monitor 464 1621;select atomno=461 or atomno=1633 or  
atomno=464 or atomno=1621;spacefill 140;select 57 and protein;wireframe off" ,"Arg57 to T4  
phosphate" , "" )</script>  
<BR>
```

```
<script> jmolCheckbox( "select all;cartoon off;spacefill off;wireframe off;backbone off;select  
protein;backbone 120;select nucleic;wireframe 80;select protein and 58;wireframe 100;monitor  
474 1668;select atomno=474 or atomno=1668;spacefill 140" ,"monitor 474 1668;select atomno=474 or  
atomno=1668;spacefill off;select protein and 58;wireframe off" ,"Arg58 to A5" , "" )</script>  
<BR>
```

```
<script> WrapUpPage() </script>  
</BODY>  
</HTML>
```

This part must be at the end.
Do not change anything.