



JMOL/JSMOL TUTORIAL

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1) DOWNLOAD JMOL APP OFF OF SOURCEFORGE

https://sourceforge.net/projects/jmol/?source=typ_redirect

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Jmol

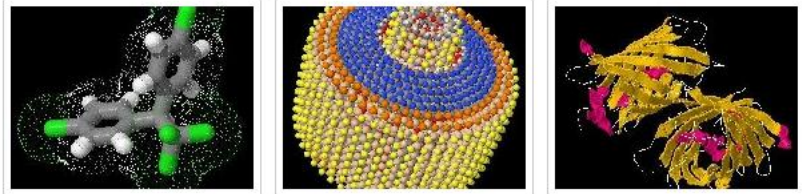
An interactive viewer for three-dimensional chemical structures.
Brought to you by: egonw, hansonr, migueljmol, nicove

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↓ 2,146 Downloads (This Week)
📅 Last Update: 2016-03-25

 **Download**
Jmol-14.4.4_2016.04.22-binary.zip




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Description

Over 10,000,000 page views! Jmol/JSmol is a molecular viewer for 3D chemical structures that runs in four independent modes: an HTML5-only web application utilizing jQuery, a Java applet, a stand-alone Java program (Jmol.jar), and a "headless" server-side component (JmolData.jar). Jmol can read many file types, including PDB, CIF, SDF, MOL, PyMOL PSE files, and Spartan files, as well as output from Gaussian, GAMESS, MOPAC, VASP, CRYSTAL, CASTEP, QuantumEspresso, VMD, and many other

Recommended Projects

-  **Avogadro**
An intuitive molecular editor and visualization tool
-  **PyMOL Molecular Graphics System**
PyMOL is an OpenGL based molecular visualization system
-  **JSmol**
JavaScript-Based Molecular Viewer From Jmol

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2) DOWNLOAD YOUR PROTEIN PDB FILE

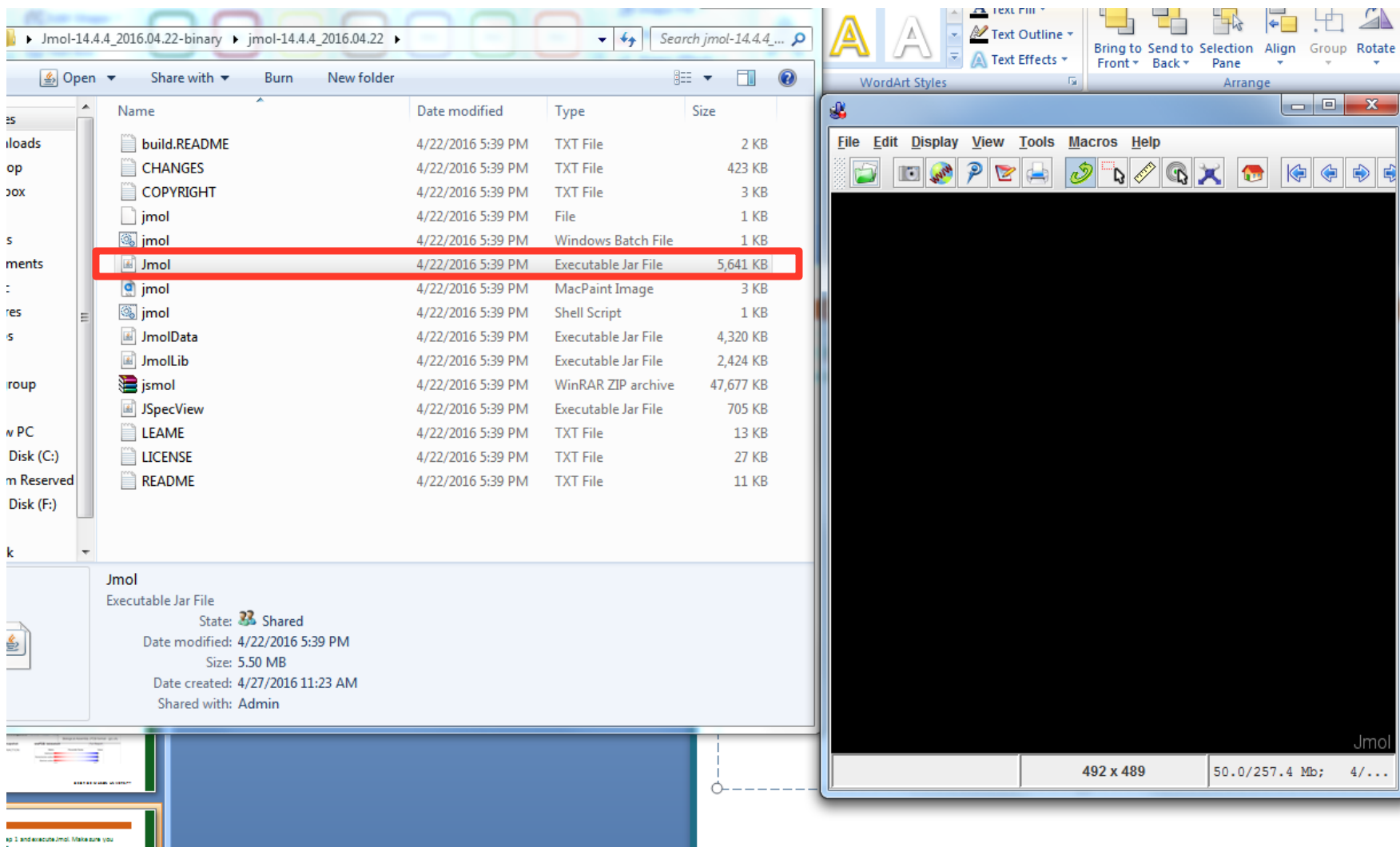
- Search for it on RCSB.

The screenshot shows the RCSB PDB website interface for protein structure 1CRN. The browser address bar displays www.rcsb.org/pdb/explore/explore.do?structureId=1crn. The navigation bar includes links for Deposit, Search, Visualize, Analyze, Download, Learn, and More, along with a MyPDB Login button. Below the navigation bar, there are logos for PDB-101, Worldwide PDB, EMDatabank, and Structural Biology Knowledgebase. The main content area features tabs for Structure Summary, 3D View, Annotations, Sequence, Sequence Similarity, Structure Similarity, and Experiment. The Structure Summary tab is active, showing a 3D ribbon diagram of the protein structure. To the right of the diagram, the protein name "1CRN" is displayed, followed by the title "WATER STRUCTURE OF A HYDROPHOBIC PI RESOLUTION. PENTAGON RINGS OF WATER CRYSTALS OF CRAMBIN". Below the title, the DOI is 10.2210/pdb1crn/pdb. The classification is "PLANT PROTEIN", deposited on 1981-04-30 and released on 1981-07-28. The deposition author(s) are Hendrickson, W.A. and Teeter, M.M., and the organism is *Crambe hispanica*. A dropdown menu is open under "Download Files", showing options: FASTA Sequence, PDB Format (highlighted with a red box), PDB Format (gz), PDBx/mmCIF Format, PDBx/mmCIF Format (gz), PDBML/XML Format (gz), and Biological Assembly (PDB format - gz) (A). Below the dropdown, there is an "Experimental Data Snapshot" section with "Method: X-RAY DIFFRACTION", "Resolution: 1.5 Å", and "R-Value Work:". To the right, there is a "wwPDB Validation" section with a "Full Report" link and a table of metrics.

Metric	Percentile Ranks	Value
Clashscore		0
Ramachandran outliers		0
Sidechain outliers		0

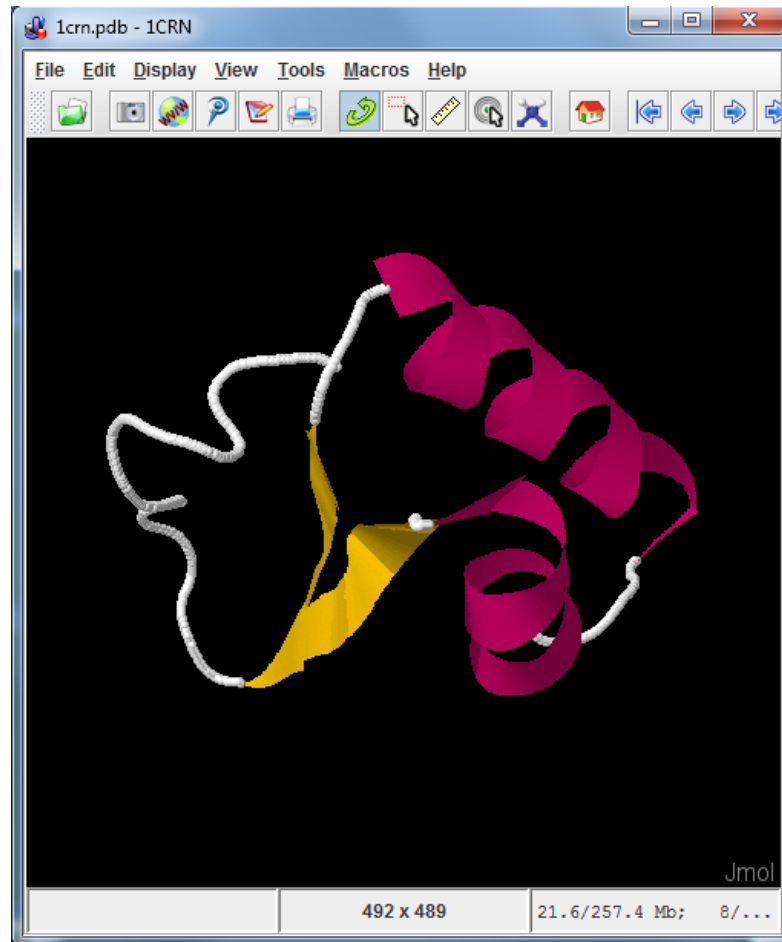
3) EXECUTE JMOL

- Unzip the jmol file you downloaded in step 1 and execute Jmol (Executable Jar File). Make sure you have Java updated to the latest version.



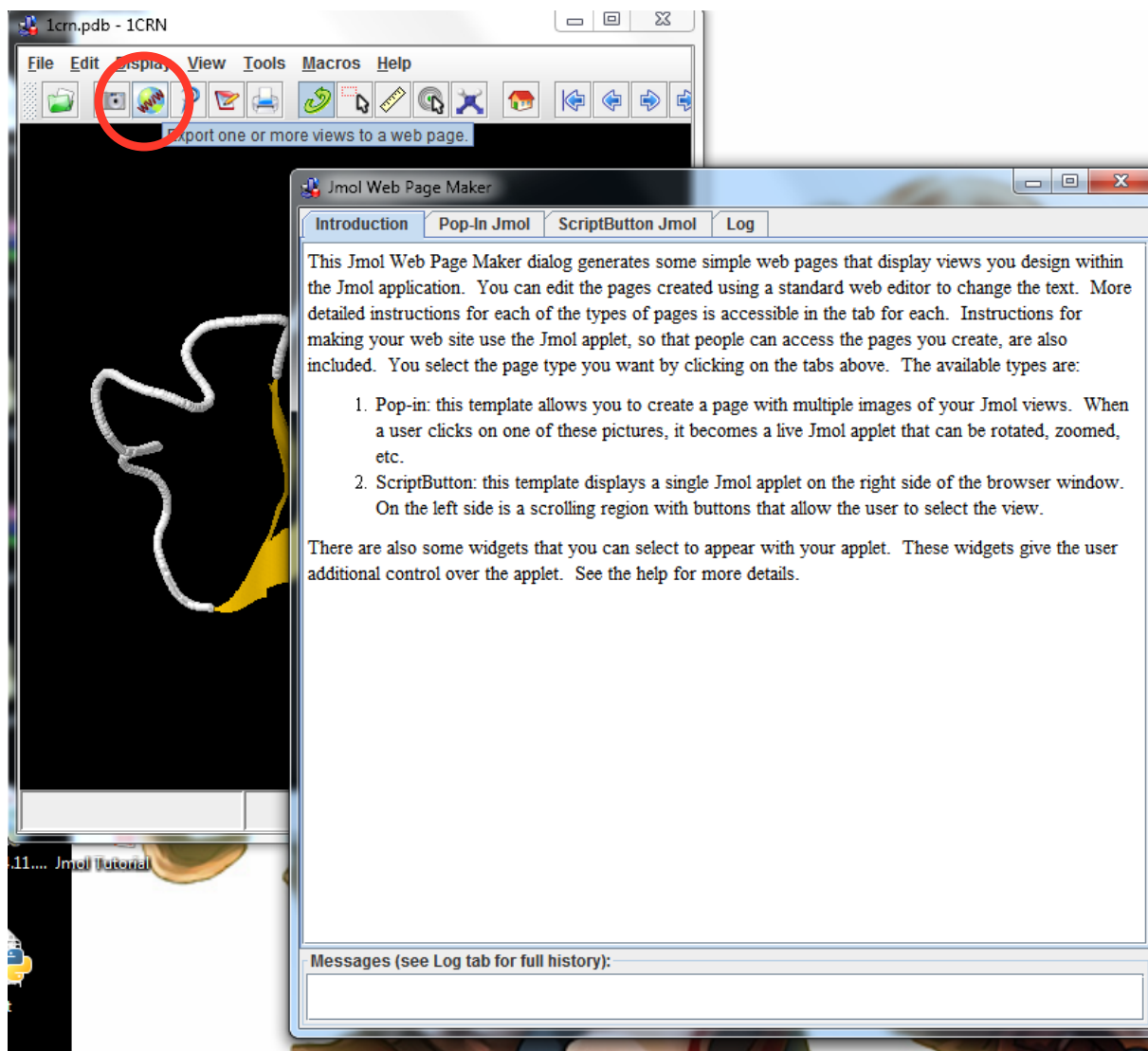
4) OPEN YOUR PDB FILE

- Select the “File” tab and click “Open”
- Navigate to where your .PDB file is saved and open it. The 3D model of the protein should appear



5) EXPORT PDB AS A WEBPAGE

- Click the little globe icon on the upper left hand corner



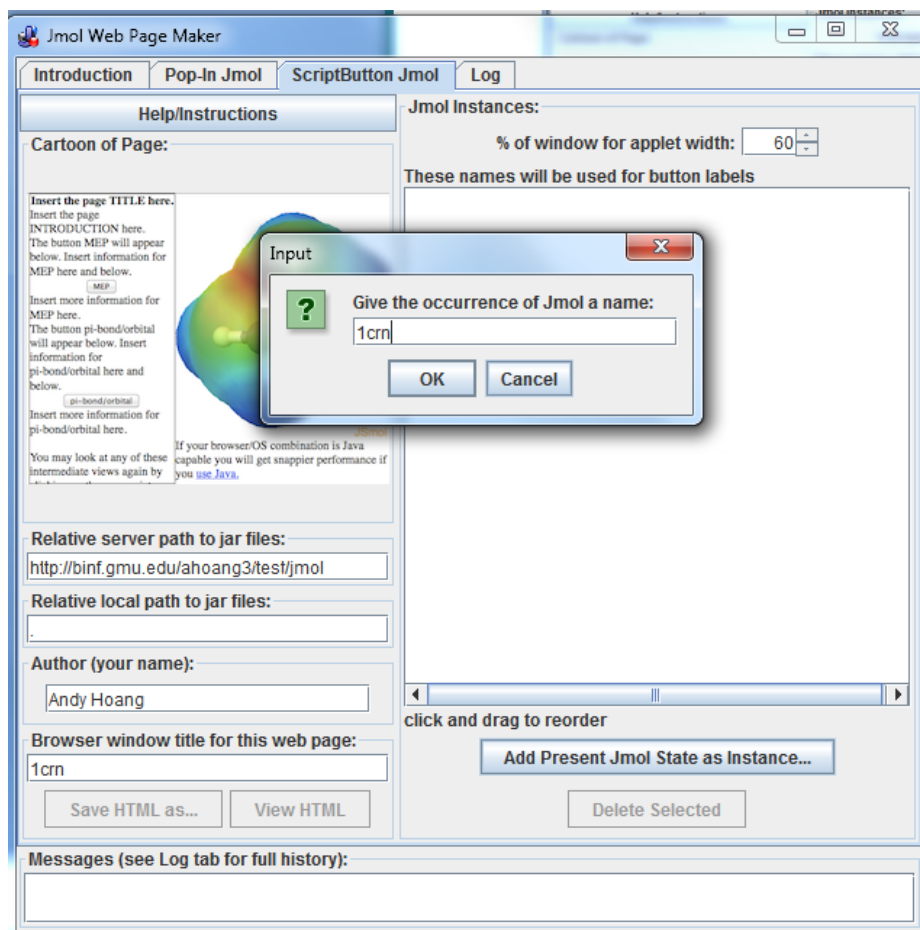
6) NAVIGATE TO SCRIPTBUTTON JMOL TAB

The screenshot shows the Jmol Web Page Maker application window. The title bar reads "Jmol Web Page Maker". The interface is divided into several sections:

- Navigation Tabs:** Introduction, Pop-In Jmol, **ScriptButton Jmol** (selected), Log.
- Help/Instructions:** A section on the left containing a "Cartoon of Page:" with a 3D molecular model and instructions for inserting page content. The model is a ball-and-stick representation with a color-coded electrostatic potential surface. Below it, there are buttons labeled "MEP", "pi-bond/orbital", and "JSmol".
- Jmol Instances:** A section on the right with a control for "% of window for applet width:" set to 60. Below this is a large empty box labeled "These names will be used for button labels".
- Configuration Fields:**
 - Relative server path to jar files:
 - Relative local path to jar files:
 - Author (your name):
 - Browser window title for this web page:
- Buttons:** "Save HTML as...", "View HTML", "Add Present Jmol State as Instance...", and "Delete Selected".
- Messages:** A section at the bottom labeled "Messages (see Log tab for full history):" with an empty text area.

7) ADD JMOL STATE

- Click “Add Present Jmol State as Instance” to save what protein jmol window is currently viewing. Name the instance and hit “Ok”
- You can even add multiple states if you wish to have a list of PDB proteins to view on your page. Simply repeat steps 2-7 for each different PDB protein



8) SAVING THE HTML (THIS IS TRICKY!!!)

- Be sure to know the URL to where your BINP files will be added for this assignment. (For example: binf.gmu.edu/ahoang3/test) Do not include “public_html”
 - If you’re not sure, check using WinSCP or a similar drag and drop tool for SSH
- In the “Relative server path to jar files” text box, input the URL to your HTML pages and add “/jsmol” to the end (<http://binf.gmu.edu/ahoang3/test/jsmol>)
 - The “s” in jsmol is important!
- “Relative local path to jar files” can be left with a “.”
- Enter the Author and Browser window title and then hit “Save HTML as...” and save it as an .html file


Jmol Web Page Maker

Introduction Pop-In Jmol ScriptButton Jmol Log

Help/Instructions

Cartoon of Page:

Insert the page TITLE here.
Insert the page INTRODUCTION here.
The button MEP will appear below. Insert information for MEP here and below.
Insert more information for MEP here.
The button pi-bond/orbital will appear below. Insert information for pi-bond/orbital here and below.
Insert more information for pi-bond/orbital here.
You may look at any of these intermediate views again by



JSmol

If your browser/OS combination is Java capable you will get snappier performance if you [use Java](#).

THIS IS IMPORTANT!!!

Relative server path to jar files:
http://binf.gmu.edu/ahoang3/test/jsmol

Relative local path to jar files:

Author (your name):
Andy Hoang

Browser window title for this web page:
1crn

Save HTML as... View HTML

Messages (see Log tab for full history):
file C:/Users/Andy_2/Desktop/asdgasdgasgasdgadgasgasg/1crn.html created

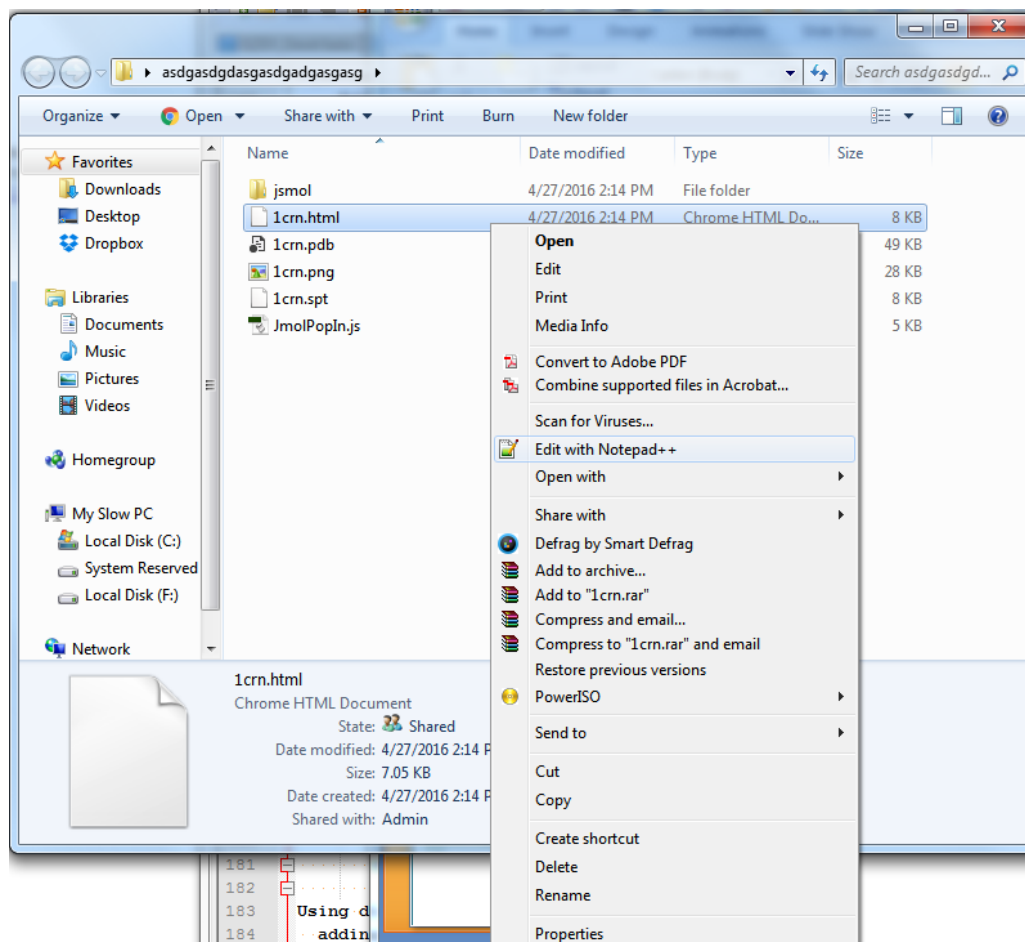
Jmol Instances:
% of window for applet width: 60
These names will be used for button labels
1crn

Select a directory to create or an HTML file to save
Save In: asdgasdgasgasdgadgasgasg
File Name: 1crn.html
Files of Type: All Files
Save Cancel

Add Present Jmol State as Instance...
Delete Selected

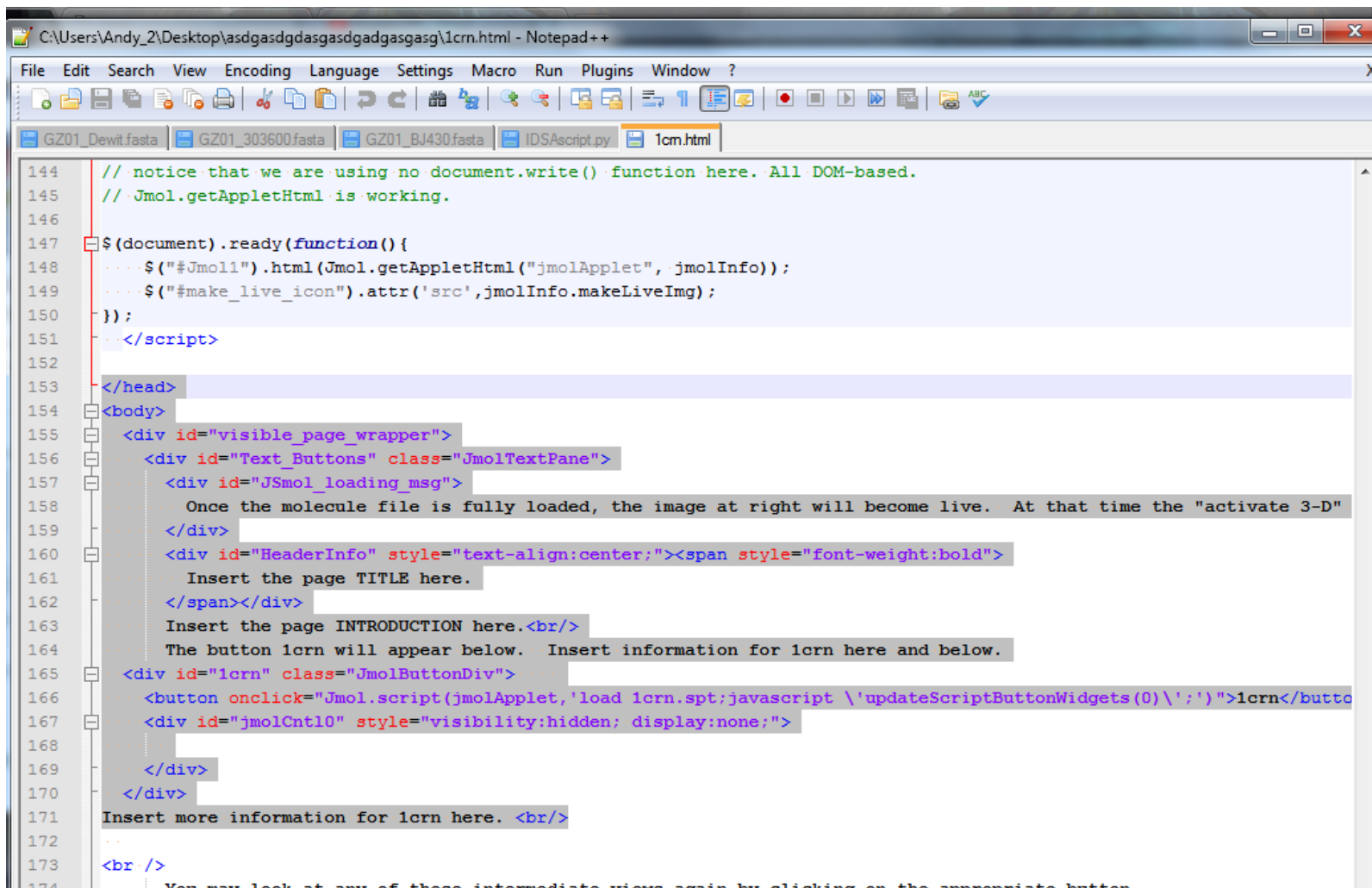
9) EDIT YOUR JMOL HTML FILE

- After you hit “Save HTML as...” an html file should generate along with the necessary jmol files to run it on your webpage.
- Manually edit the html file using a text editor, such as Notepad++ or TextWrangler.



HTML EDITING CONTINUED

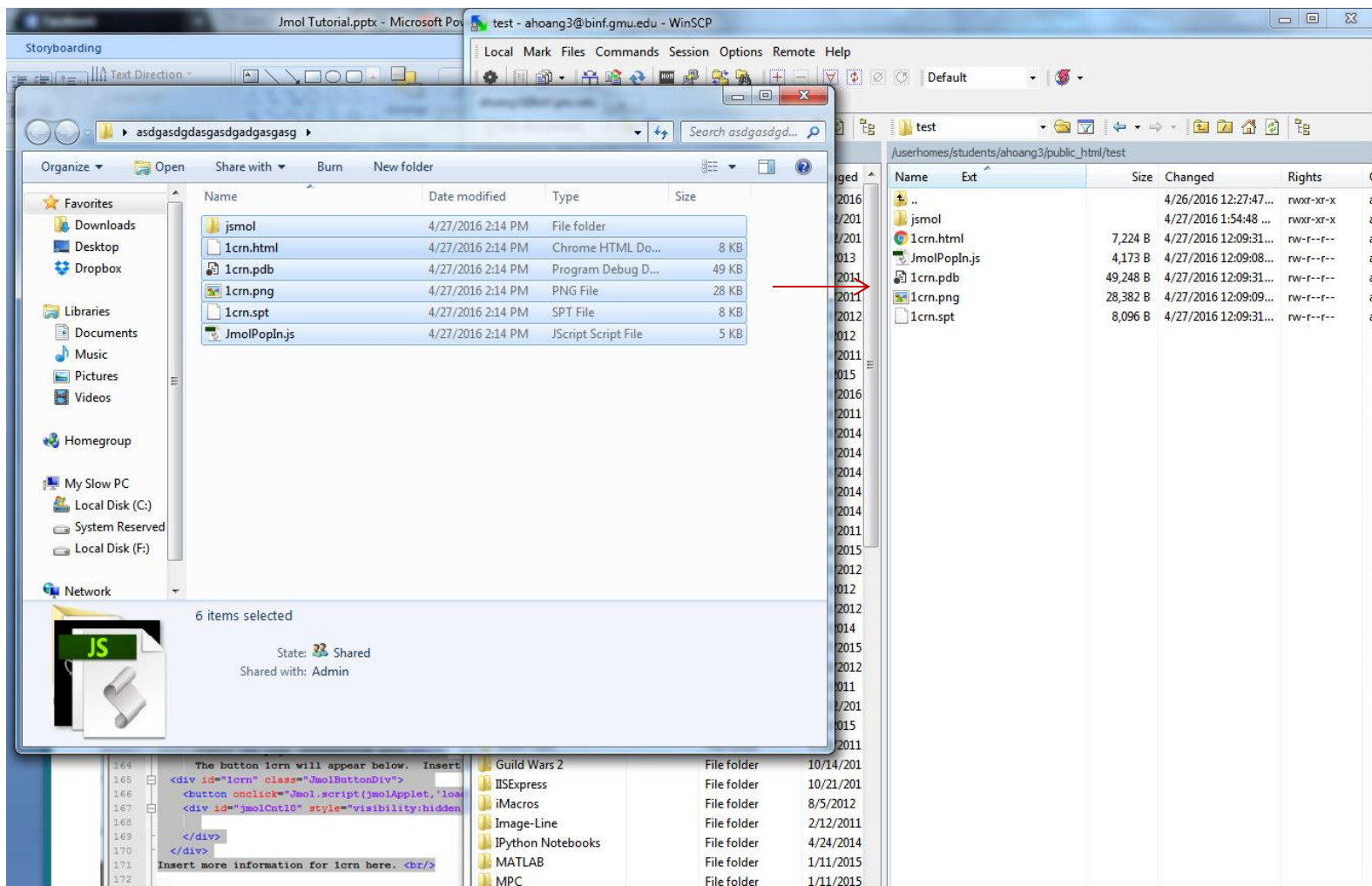
Scroll down and find this section of code. This is where you can edit for more details on your PDB file. Don't edit anything else unless you know what you're doing. Save when done.



```
144 // notice that we are using no document.write() function here. All DOM-based.
145 // Jmol.getAppletHtml is working.
146
147 $(document).ready(function(){
148     $("#Jmol1").html(Jmol.getAppletHtml("jmolApplet", jmolInfo));
149     $("#make_live_icon").attr('src', jmolInfo.makeLiveImg);
150 });
151 </script>
152
153 </head>
154 <body>
155     <div id="visible_page_wrapper">
156         <div id="Text_Buttons" class="JmolTextPane">
157             <div id="JSmol_loading_msg">
158                 Once the molecule file is fully loaded, the image at right will become live. At that time the "activate 3-D"
159             </div>
160             <div id="HeaderInfo" style="text-align:center;"><span style="font-weight:bold">
161                 Insert the page TITLE here.
162             </span></div>
163             Insert the page INTRODUCTION here.<br/>
164             The button 1crn will appear below. Insert information for 1crn here and below.
165             <div id="1crn" class="JmolButtonDiv">
166                 <button onclick="Jmol.script(jmolApplet, 'load 1crn.spt;javascript \'updateScriptButtonWidgets(0)\';')">1crn</butto
167             <div id="jmolCntl0" style="visibility:hidden; display:none;">
168
169             </div>
170         </div>
171         Insert more information for 1crn here. <br/>
172     </div>
173 </br />
174     You may look at any of these intermediate views again by clicking on the appropriate button
```

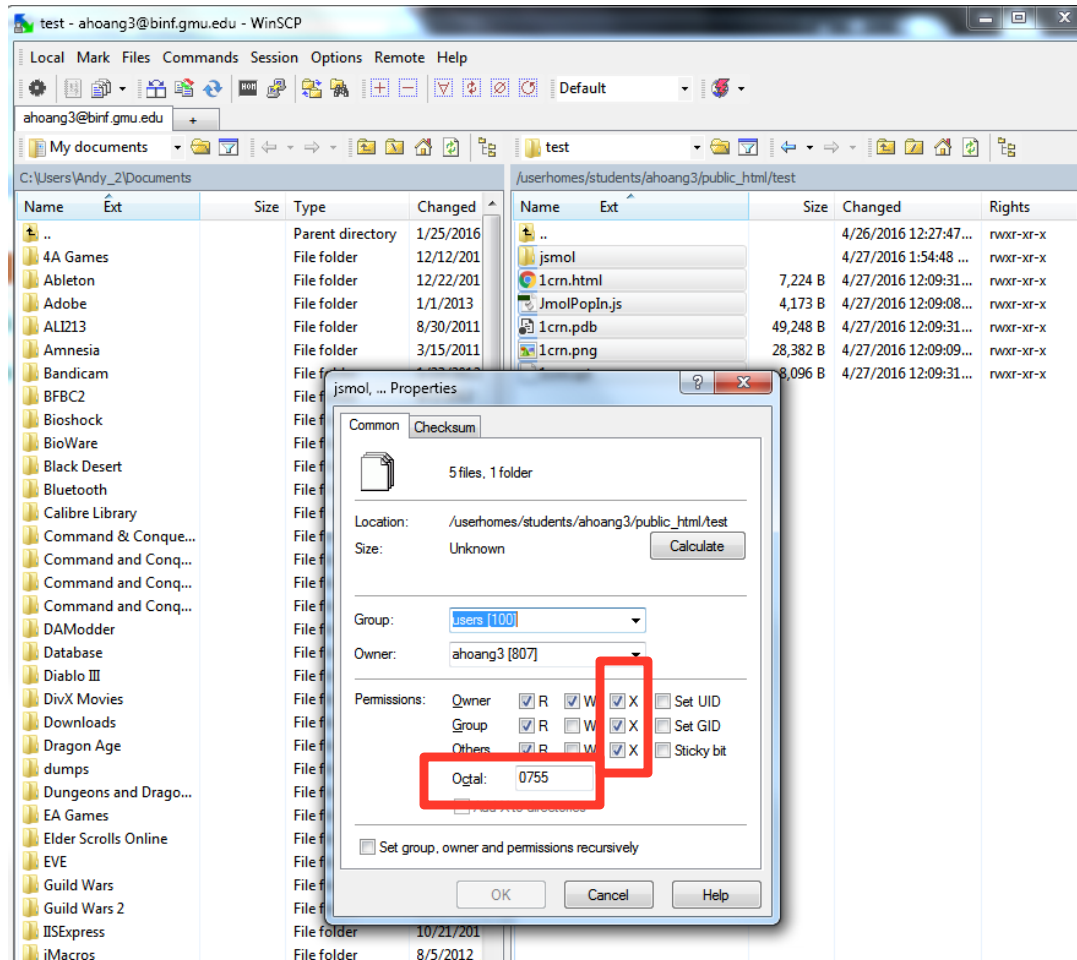
10) TRANSFER FILES TO BINP

- Transfer all your files to your binp server and where your project is stored using WinSCP or an equivalent program



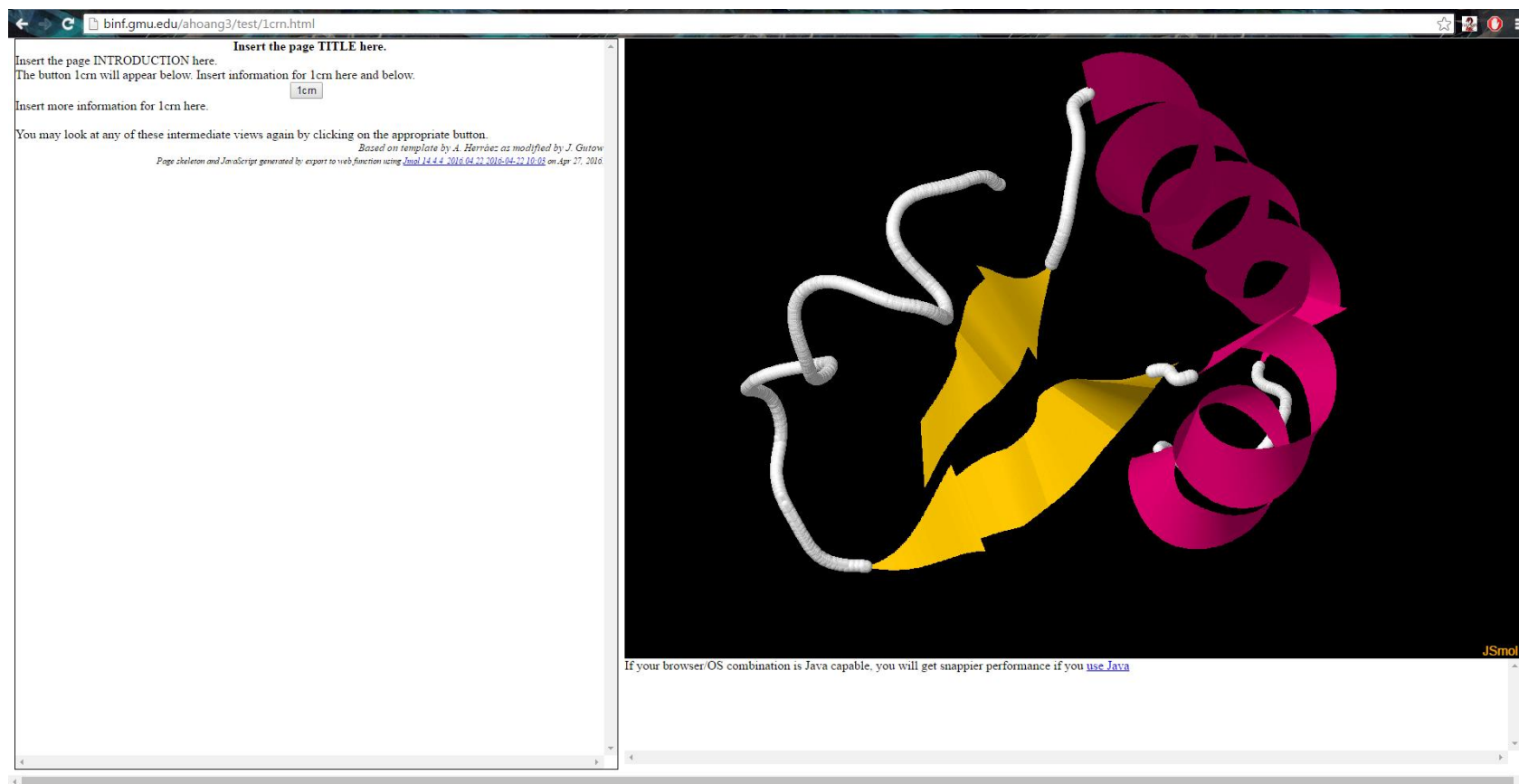
SET ALL FILES TO BE EXECUTABLE

- Highlight over all your files and click “Properties”
- Set all of the permissions to be exactly like the image below or manually type “0755” as the octal. Hit OK when finished



11) CHECK TO SEE IF THE PAGE IS WORKING

- Type the URL of where the jmol html file is stored. For my file, it was: <http://binf.gmu.edu/ahoang3/test/1crn.html>
- Check to see if it runs. If it does, yay! If not, double check the steps above and retry...



The screenshot shows a web browser window with the address bar containing the URL binf.gmu.edu/ahoang3/test/1crn.html. The page content includes instructions for inserting a title and introduction, a button labeled "1crn", and a 3D molecular structure visualization. The structure is rendered in a ribbon style, showing a yellow beta-sheet and a magenta alpha-helix. The browser window also displays a footer with the text "JSmol" and a note about Java performance.

Insert the page TITLE here.

Insert the page INTRODUCTION here.
The button 1crn will appear below. Insert information for 1crn here and below.

Insert more information for 1crn here.

You may look at any of these intermediate views again by clicking on the appropriate button.

Based on template by A. Herráez, as modified by J. Gutov
Page skeleton and JavaScript generated by export to web function using Jmol 14.4.4 2016-04-22 2016-04-22 10:02 on Apr 27, 2016

JSmol

If your browser/OS combination is Java capable, you will get snappier performance if you [use Java](#)

CONTACT

Feel free to email me any questions or concerns:
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