Exploring Protein structures from the Protein Data Bank using JSmol Webpages

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DOWNLOADS & INSTALLATION

You do not need to install any software to view/edit interactive Jmol figures online.

If you want to make your own Jmol figures from scratch you will need to install the standalone Jmol application jmol.jar. (Download the Jmol package (either .zip or tar.gz format) and extract/uncompress **only the** **Jmol.jar file** to the folder of your choice. See http://wiki.jmol.org/index.php/Jmol_Application#Installing_Jmol_Application). It may be useful to put a shortcut to this file on your desktop.
The standalone application requires Java to be installed on your computer (this is not the case for viewing jmol webpages). Download from https://java.com/en/download/manual.jsp and install.

Double-click on the Jmol.jar applet or shortcut to open the program.

(To use all the full range of the Jmol app you should install the full system – only do this if you find you want something not available in the standalone app.)

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MANIPULATING JSMOL FIGURES

Some general comments and some common operations follow, you can also consult the Jmol/JSmol Scripting Documentation, and the Jmol/JSmol Wiki. These instructions assume you are using the standalone app – there are a few differences if you are using another method.

The Jsmol logic is that you ***select*** part of the structure and then apply some change to the selected part. There are 2 ways to make a selection:

1) Right-click somewhere in the graphics box and click on "**Select**" in the menu, then click through the sub-menus as required
2) Right-click in the graphics box and click on "**Select**" in the menu, then choose "**Console**". In the Console box, type "select *name"* where *name* = e.g. "protein", or "copper" or "atomno=1256" or "His87" etc followed by "↵" (ie "enter" or "return").

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Option (1) is fine for basic operations, option (2) is more flexible – and often much quicker.
It is sometimes helpful to highlight your selections – right-click in the graphics box, click "**Select**", click "**Selection Halos**".
To reset the selection via the console type "**select all**"

EXAMPLES
Note: **commas** are used to separate items in a list of selections and a **semi-colon** (**;**) is used to separate commands typed into the console. Alternatively, you can type each part, then "↵" (ie "enter" or "return"). Red text in the console indicates incomplete or incorrect syntax.

Change background colour:

either Right-click in the GUI, select "**Color**", then "**Background**", then e.g. "**White**"
or In the console type "**background white**"

Identify an atom or amino acid
Place the cursor over the atom, a label will appear eg "**[HIS]245:A.ND1 #1585**". This is a nitrogen atom at the D1 position of Histidine 245 in chain A and it is atom number 1585 in the atom list.

- This atom It can be referred to as "**atomno=1585**", "**nitrogen**" refers to all nitrogen atoms in the current selection
- The histidine can be identified as "**his345**", "**his**" refers to any histidine in the structure
- "**:A**" refers to all atoms in chain :A

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Hide subunits B, C and D

In the console type "**select :B, :C, :D; hide selected**"
Note: you can only have one set of hidden objects – so if you want to hide e.g chlorine as well type "**select :B, :C, :D, chlorine; hide selected**"

Hide water molecules

either Right-click in the GUI, select "**Select**", then "**Hetero**", then e.g. "**All water**"
or In the console type "**select water; spacefill 0**"

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Zoom

either Right-click in the GUI, select "**Zoom**", then click on a value in the drop down menu (100 is the original value)
or In the console type e.g. "**zoom 200**"

Centering

either Click on the centering icon (10th in the row above the graphics box, click on the atom you wish to center on.

or In the console type e.g. "**select atomno=1897; center selected**"

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Change size, colour of atoms

either Right-click in the GUI, select "**Select**", then "**Hetero**", then "**By HETATOM**", then e.g. "**Copper**". Right-click in the GUI, select "**Color**", select "**Atoms**", select "**Green**". Right-click in the GUI, select "**Style**",then select "**Atoms**", then select "**75% van der Waals**".

or In the console type "**select copper; color green; spacefill 75%**"

Show the protein as a cartoon and colour it by secondary structure

either Right-click in the GUI, select "**Select**", then "**Protein**", then "**All** ". Right-click in the GUI, select "**Style**", then select "**Structures**", then select "**Cartoon**". Right-click in the GUI, select "**Color**", then select "**By Scheme**", then select "**Secondary structure**".

or In the console type "**select protein; spacefill 0; wireframe 0; cartoon on; color structure**"

To remove the cartoon

either Right-click in the GUI, select "**Select**", then "**Protein**", then "**All** ". Right-click in the GUI, select "**Style**", then select "**Structures**", then select "**Off**".

or In the console type "type: "**select all; cartoon off**"

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Show all the amino acid residues as thin lines with CPK colours

either Right-click in the GUI, select "**Select**", then "**Protein**", then "**side-chains**". Right-click in the GUI, select "**Style**", then select "**Bonds**", then select "**0.10A**". Right-click in the GUI, select "**Color**", then select "**By Scheme**", then select "**Element (CPK)**".
(to hide the side chains again repeat the sequence replacing "**0.10A**" by "**off**")

or In the console type "**select sidechains; wireframe 10; color cpk**"
(to hide the side chains again repeat the sequence replacing "**10**" by "**0**")

Make object translucent

In the console type e.g.

"**select all; color cartoon translucent 0.5**" or
"**select zinc; spacefill 200; color translucent blue** "

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Show selected amino acid chains as sticks with CPK colours bonded to a metal ion

In the console type e.g. "**select His238, Tyr98, asp283, atomno=1854; wireframe 50; color cpk**" where 1854 is the sequence number of the metal ion.

Connect two atoms

In the console type e.g. " **connect (atomno=1) (atomno=2)**"

Unbond two atoms

In the console type e.g. " **connect (atomno=1) (atomno=2) delete**"

Add a (dashed) hydrogen bond between two atoms

In the console type e.g. " **connect (atomno=1) (atomno=2) hbond**"

Hbond style: connect (atomno=571)(atomno=10741) hbond radius 0.1 modify

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EXPORTING FIGURES

The png format gives good resolution graphics files which are not too large. To generate a *name*.png figure showing the current state: Right-click in the graphics box, click on "**File**", then "**Export**", then "**Export png image**". A new box will open; navigate to the directory where you want to put the saved script, change the name if you wish (but ***keep*** the *.png suffix) then click "**Save**".

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"All care, no responsibility"- VMcK