Northwestern University Feinberg School of Medicine

Galter Health Sciences Library & Learning Center

Structure Viewers

Take a Class

This guide supports the Galter Library class called **Structure Viewers**. See our Classes schedule for the next available offering. If this class is not on our upcoming schedule, it is still available to you or your group by request.

Uses for Structure Viewers

There are many software packages for viewing molecular structures available for purchase or as free software downloads on the Web. Some structure viewers are good for viewing individual or multiple structures, while others provide more options for analysis of structure features. Others are best for creating publication-quality images.

This guide demonstrates the use of two structure viewers: NCBI's Cn3D and SwissProt's Deep View (also known as SPDBV). Users will learn where to download both viewers, how to use them for aligning similar structures, how to import a sequence to align to a structure and how to edit a structure's displayed characteristics.

The beginning of this guide offers a brief introduction to the Protein Data Bank, where users can download structure files.

The end of this guide provides users a link to download Pymol, a structure viewer that creates excellent publication-quality images. A list of other structure viewers is also located at the end of this guide.
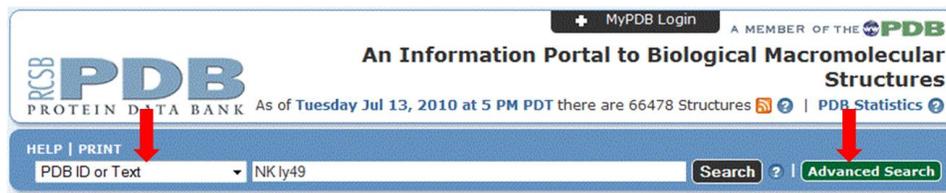
Finding Structures at the PDB

The Protein Data Bank (PDB) is the official world wide repository for molecular structures.

Search the PDB by

- Text keyword (such as a description of the molecule)
- PDB identifier
- Author name
- Chemical name
- Chemical identifier

This guide uses the example of "NK ly49" to search for natural killer receptor Ly49.

You can also click on the **Advanced Search** button and perform a guided search by specific field in the PDB record. The advanced search is also where you can paste a sequence and perform a BLAST against the structures in the PDB to see if a structure exists with similarity to your sequence.

In your search results page, you can **refine** your results by removing redundant structures using options to decrease sequence similarity. You can also **sort** your results by

- PDB identifier
- Release date (this is the default display)
- Residue count
- Structure resolution

Select a structure record by clicking on the PDB identifier or the description of the structure.

On the PDB structure summary

- View summarized details of the structure, such as release publications, species information, chain information
- Use the **tabs** at the top of the page to view detailed information on protein families, experimental conditions and geometry or perform sequence or structure similarity searches
- View **images** of the structure
- Use PDB's options of structure **viewers** to see your protein. Jmol is the recommended default.
  - Note: Jmol is a Java-based application and will open in your browser window. Jmol is a very user-friendly application and allows you to view the structure in many ways. Users are encouraged to explore the features of Jmol, since this guide does not cover this viewer.
- **Download** files using the links near the upper right of the summary page (next to the PDB identifier)
  - The drop-down Download menu offers many options for file formats. Usually the .pdb files will be the most compatible with most structure viewers, but other formats are available.

NCBI's Structure Database and Cn3D

Structures can be searched in other databases besides the PDB. You can search for structures at the NCBI, as well. Cn3D is a structure viewer created by the NCBI. It is the default structure viewer for opening structures from NCBI's Molecular Modeling Database (MMDB).

To use Cn3D, you must first download the software onto your computer. Download links for Cn3D are located at multiple places in the structure search results, structure summary pages and from the NCBI's structure home page. Here is a direct link to the Cn3D download page.

- On the NCBI home page, use the pull down menu above the search box to select **Structure**
- Type your search terms in the box
  - Again, this example uses NK ly49
  - You can also search by PDB identifier number, if you know it
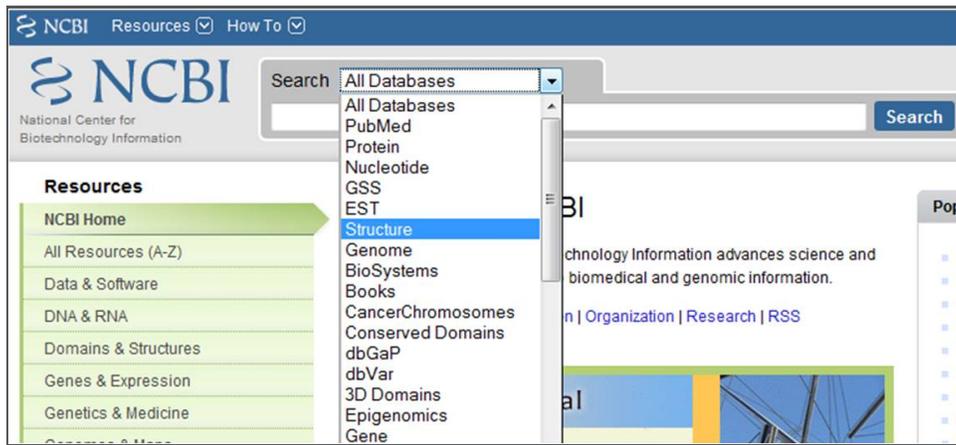
Your search results page will display thumbnail images and summaries of all results.


From the results page, you can

- Refine your search using **limits**
- Link to protein **families** or **superfamilies**
- Link to **literature** citing the structure
- See if your results include heterogeneous structure **complexes**
- See **species** distribution of results
- Use the **links** to related structures, domains and other links
- **Click** on the **PDB identifier** to view an individual record (this example uses 1P1Z)

From the structure summary page, you can click on the image of the structure to open it with Cn3D (if you have Cn3D installed on your computer--if not, you will be directed to the Cn3D download page).

For chain-specific structure comparisons, scroll down the page to the section showing the structure domain schematic images.
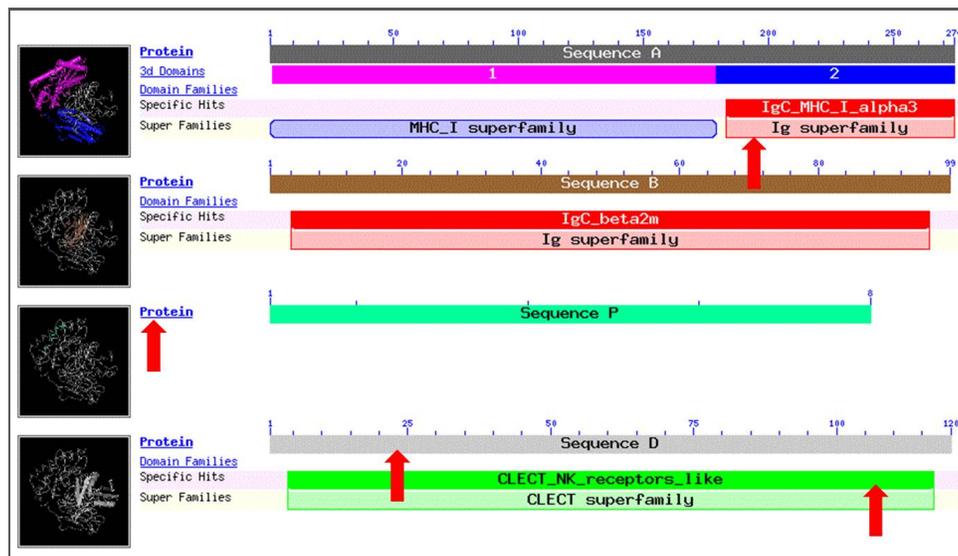
From this view you can

- Link to the protein records using the **Protein** links
- Click on the colored bars to access records in NCBI's Conserved Domains Database for **families** and **superfamilies**
    - Families are shown in darker colors and are located above superfamilies
    - If a chain of your structure contains more than one domain, all domains will be arranged along the sequence bar
- Click on the **Sequence** bar to access an alignment of structures that have similarity to that particular chain

For this example, click on the Sequence D bar.

NCBI's VAST Related Structures

You are now on a page showing results from NCBI's VAST (Vector Alignment Search Tool) Related Structures search. On this, you will see a number of red bars aligned to your query sequence graphic. The results of this search are not limited to a specific family (such as natural killer cell receptors in this example) but will likely suggest members of a related fold class or superfamily.

To display multiple structures aligned to each other, click the **checkboxes** next to a few of the VAST results (the limit is 9) and click the **View 3D Alignment** button at the top of the page.

Viewing Structures with Cn3D
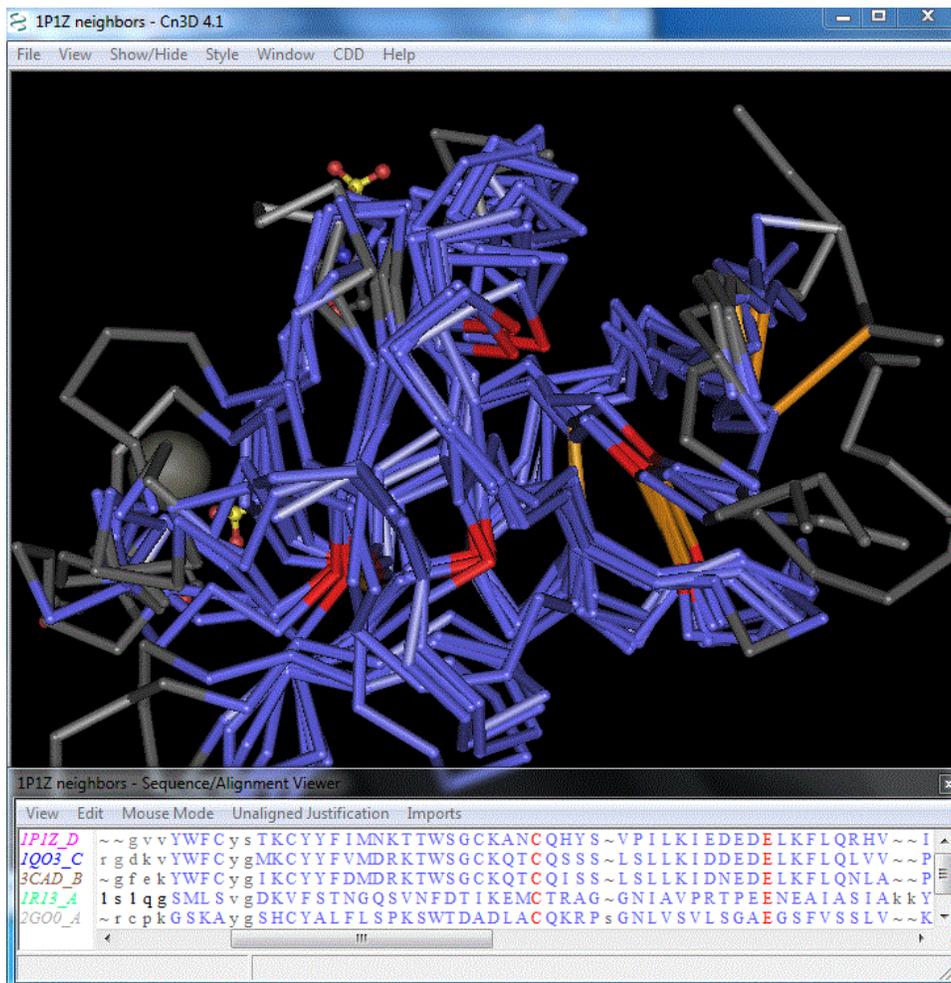
You are now viewing a multiple structure alignment in Cn3D. Cn3D will open two windows: a structure view window and a sequence view window. The style of the molecules is different from what you would see by opening any individual structure directly from its Structure Summary page at NCBI. The color shown is based on identity of amino acids, with red representing identical residues across the structures and cooler colors (such as blue) representing less similar amino acids. Note that, despite the low degree of sequence identity, the structural alignment is fairly good.

With Cn3D you can modify the view of your structure(s) in many ways:

- Click and drag your mouse on the structure view to **rotate** the molecule(s)
- Hold down the **Shift** key and click and drag your mouse to slide the molecule(s)
- Hold down the **Control** key and click and drag your mouse to **zoom** the structure(s) in or out

- **View** menu
    - **Zoom** in or out
    - **Reset** the view or **restore** it to its original view
    - View each **frame** separately (with a multiple structure alignment, each frame is an individual structure
    - Play an **animation** of the frames
- **Show/Hide**
    - **Pick** individual structures or chains from structures
    - Show **everything**
    - Show **aligned domains** (the default view when opening Cn3D from a VAST page)
    - Show **aligned** or **unaligned residues**

- Show **selected residues** or **domains** (you need to select them from the image or the sequence window)
- Show structural features within a certain angstrom **distance**
- **Style**
  - Edit the **global style**
    - Within this pop-up window, you can change how features are shown or colored, as well as change the background
  - **Favorites** (only works if you have created a custom style and want to use it)
  - **Rendering** Shortcuts
    - Worms (the default style if you are viewing an individual structure)
    - Tubes (the default if you are viewing an alignment)
    - Wire
    - Ball and stick
    - Space fill
    - Toggle side chains (to be visible or invisible)
  - **Coloring** Shortcuts
    - Secondary structure (the default if you are viewing an individual structure)
    - Aligned
    - Sequence conservation
      - Identity (the default if you are viewing a multiple structure alignment)
      - Variety or weighted variety
      - Information content
      - Fit
    - Object (each structure is an object)
    - Domain
    - Molecule (each type of molecule in a class will be the same color)
    - Hydrophobicity
    - Charge
    - Temperature
    - Element
  - Annotate to create your own custom style for a highlighted section
- **Window** - allows you to display or hide the sequence viewer and message logs
- **CDD** - only available if you have opened a family from a CDD page
- **Help**

From the **Sequence/Alignment** view window

- **View menu**
  - PDB titles (default)
  - Geometry violations
  - Find a specific Prosite pattern
  - View or hide rows
  - Show a Position-Specific Scoring Matrix (PSSM) score upon mouse-over
  - Show self-hits from database similarity scores
  - Export sequence alignment in FASTA or other formats
  - Show a taxonomy tree
- **Edit**
  - Enable or disable the editor (you must enable the editor to make changes from the Edit menu)
  - Manipulate blocks by splitting or merging
  - Sync sequence colors to structure colors
  - Sort or delete rows
- **Mouse mode** - choose to select sequences by rows, columns, click-and-drag horizontal boxes (default)
- **Unaligned justification**
- **Imports** - manage an import wizard so you can import other structures or sequences
  - Click **Show Imports** in the Imports menu

- Now click on **Edit** and pull down to **Import Structure** or **Sequence**
- Now you can import a file from your computer or use the **Via Network** option to search NCBI for a structure
  - The drawback here is that you must know the MMDB ID number from the NCBI's MMDB, and you can't use a PDB identifier
  - Try importing structure number 12071
- You may have to do some editing of your imports to get them to fit your current structure
  - From the **Alignments** menu in the **Imports** window, select **Block Align Single** and click on the sequences to align
  - A new window will open
  - Click **OK**
  - Now from the **Alignments** menu, click on **Merge All**
  - Now close Cn3D but reply **Yes** to all of the save prompts and save your new file to your desktop
  - Now re-open the saved file. Some error messages may pop up, but your alignment should be visible. If it's not, go to the **File** menu in the structure viewer and choose **Realign structures**
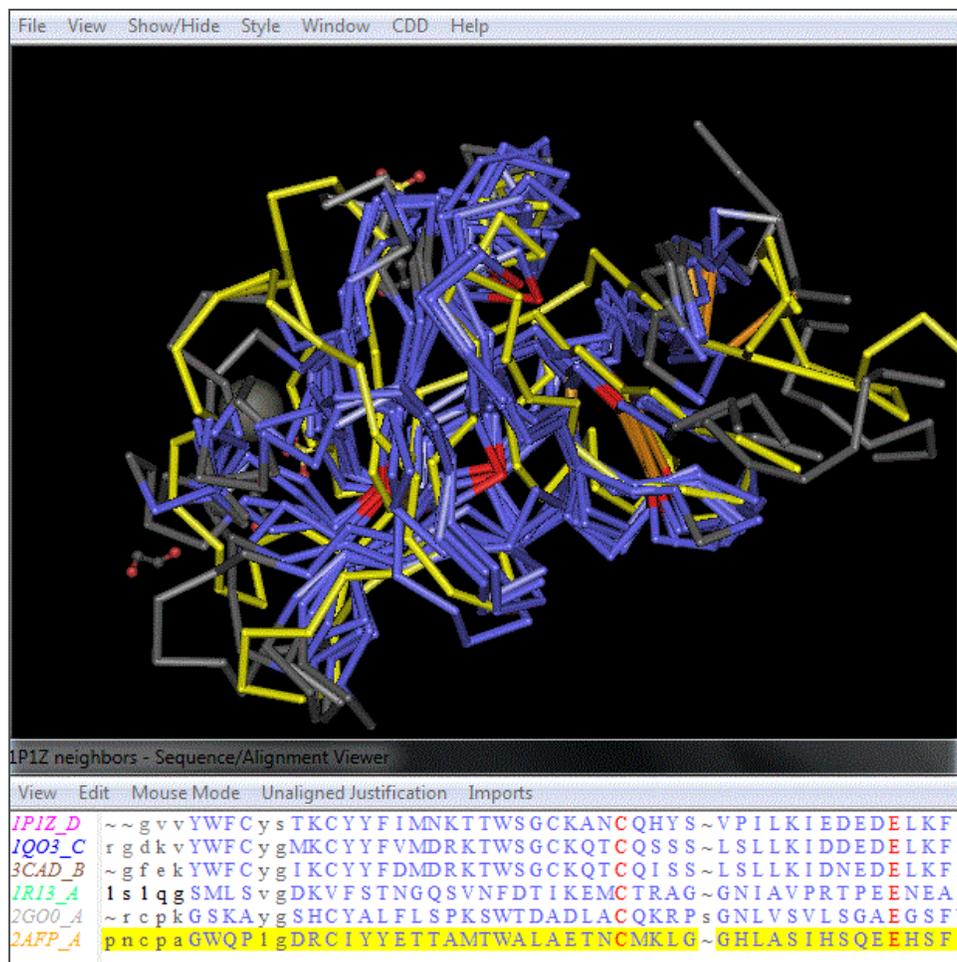
Above is a screen shot of the new alignment with the new structure added and highlighted in yellow.

Cn3D produces decent quality images, so you can export your images by going to the **File** menu and selecting **Export PNG**.

The Swiss Protein Data Bank Viewer (SPDBV) DeepView

Also known as Swiss-PDB Viewer.

DeepView has an interface that allows the user to make measurements, compute energy and change the structure of a molecule.

To download Deep View to your computer, go to the [Deep View home page](#) and select Download from the left menu bar. You will have to agree to terms of use to download the software. The software is downloaded as a zipped file, so you will have to unpack the zip file and save it to your computer's Program Files (or Applications for a Mac). Be sure to create a short cut to the program on your computer's desktop or in another location where you can find it easily.

Importing Structures to SPDBV

Open DeepView. You can close the About window so you only see the toolbar when you open the program. From the **File** menu, you can open any .pdb, mmcif or MOL (SDF) file that you have saved on your computer.

You can also use the **Import** command to search your computer for PDB files. The import window also allows you to use an Internet connection to search PDB for a particular PDB identifier. You can also search for PubChem IDs or paste a sequence in the window to model.
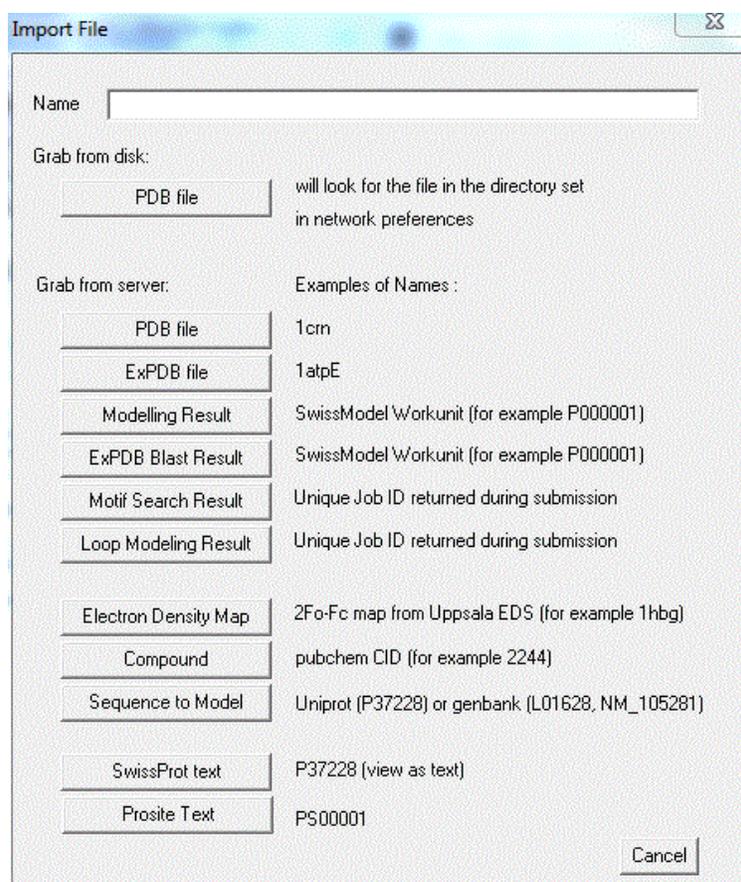
When you import a structure, sometimes structural data is incomplete, so Deep View will attempt to create side chains or other missing data. If this happens, a dialog window will open showing you all of the edits that the program made. You can close this window after viewing the information.

For this guide, use the PDB identifier 1P1Z and click the **PDB file** button in the **Grab from server** section of the menu. This is the natural killer cell receptor Ly49.

The Menu Bar in SPDBV
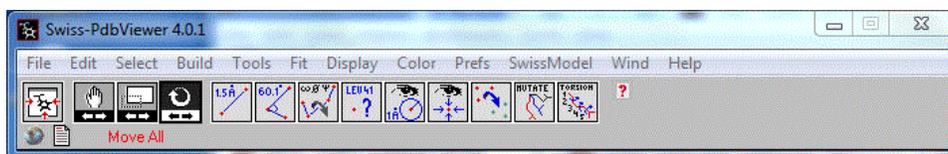
The pull-down menu bar in Deep View contains many options. There are too many options to list separately in this guide, so only a few will be demonstrated, but you can explore more functions as you become more familiar with the viewer.

The quick options are displayed as picture icons in the menu bar. These are some of the frequently-used features of the browser.

- Center - Click this to re-center your structure after resizing the window or adding more structures

- Drag - Click this to use your mouse to drag your structure on the page without rotating it

- Zoom - Click this to use your mouse to zoom in or out

- Rotate - This action is the default when you open Deep View, but you can click on this after using the drag or zoom buttons to return to rotate action mode

- Measure - Click this button, then use your mouse to click on any two atoms in your structure to measure the distance between them

- Angle - Click this button, then use your mouse to select three atoms on the same side chain or portion of the backbone to measure the angle between them

- Dihedrals - Click this button, then click anywhere on a particular amino acid to view its phi, psi and omega angles

- Provenance - Click this button, then click on an atom to display its molecule, group, chain and atom

- Display or hide a group of atoms that are a specified distance from a selected atom

- Center the view on a selected atom

- Click this button to fit a molecule to another one (only available when more than one molecule is on the screen)

- Mutate - Click this button, then select an amino acid. A menu will open that will allow you to select another amino acid to mutate to, along with an option to predict the probability that this mutation will preserve the secondary structure

- Torsion - Click this button, then select an angle on a side chain or the backbone of the molecule. You can then rotate any portion of the structure from that point to the C-terminus. You will also be warned of potential steric clashes resulting from torsional rotation.

For more detailed descriptions of these quick button options, view the help document which can be accessed by clicking the small question mark (?) next to the buttons.

After you have opened a structure, open the **Control Panel** by selecting the **Wind** menu then selecting **Control panel**. From the control panel, you can make changes to entire chains or whole structures by using the columns.

The default structure view is a wire structure, so to view either space fill or ribbons, use the columns marked **::v** or **ribn** to change the view. You can then set preferences for the ribbons using the **Prefs** menu in the viewer window.

Aligning Structures in Deep View

Import a second structure into your window using the **Import** option in the **File** menu. Try importing the PDB ID 1GZ2. This is a chicken egg shell protein (*not* a natural killer cell receptor).

When working with two or more structures, each structure is in a separate layer in the display. Toggle between layers by clicking on the structure ID in the control panel and switching to another layer by clicking its identifier.

To make your alignment easier to interpret, color the two structures by layer. In this view, 1P1Z is yellow and 1GZ2 is blue.
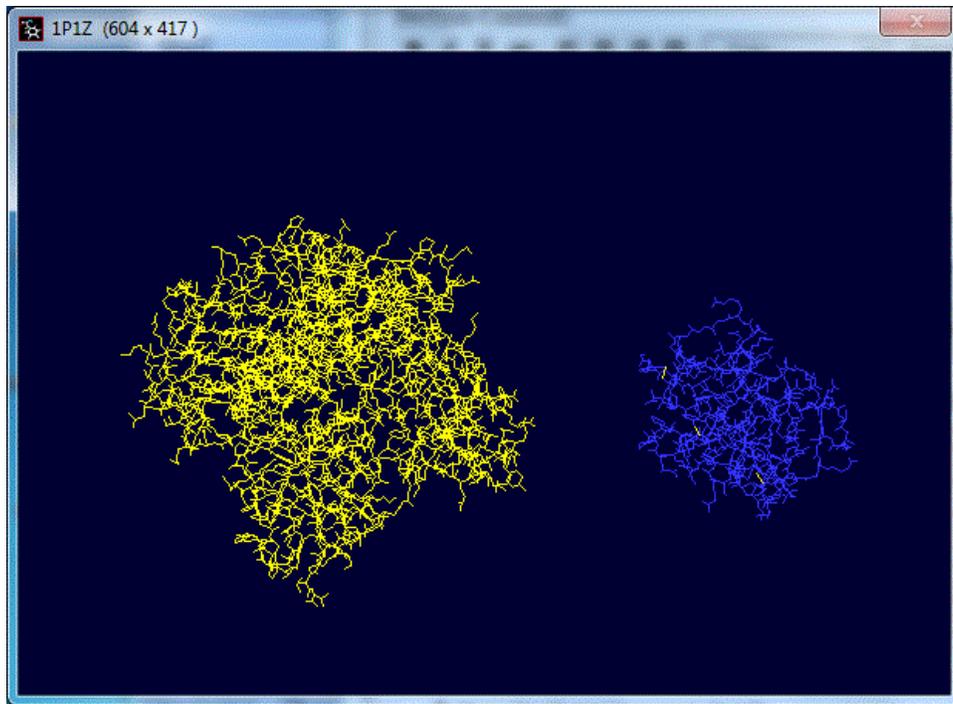

To align structures, you can use the button in the menu bar, but a better way to generate a structural alignment is to use the **Fit** menu.

- **Magic Fit** will provide a good, fast fit for somewhat similar structures
- **Iterative Magic Fit** moves through the structures adjusting the alignment iteratively
- **Explore Fragment** or **Explore Domain Alternate Fits** will perform more slowly than the Magic Fits, but may work for structures that share only small regions of structure similarity

Select **Magic Fit**, and a dialog box will pop up.
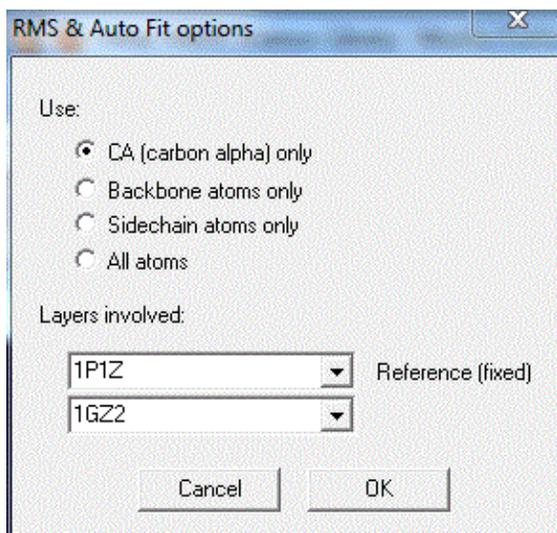
You can choose what parts of the structures to align, and which structure will be the reference layer. Click **OK**. Now your structures will align.
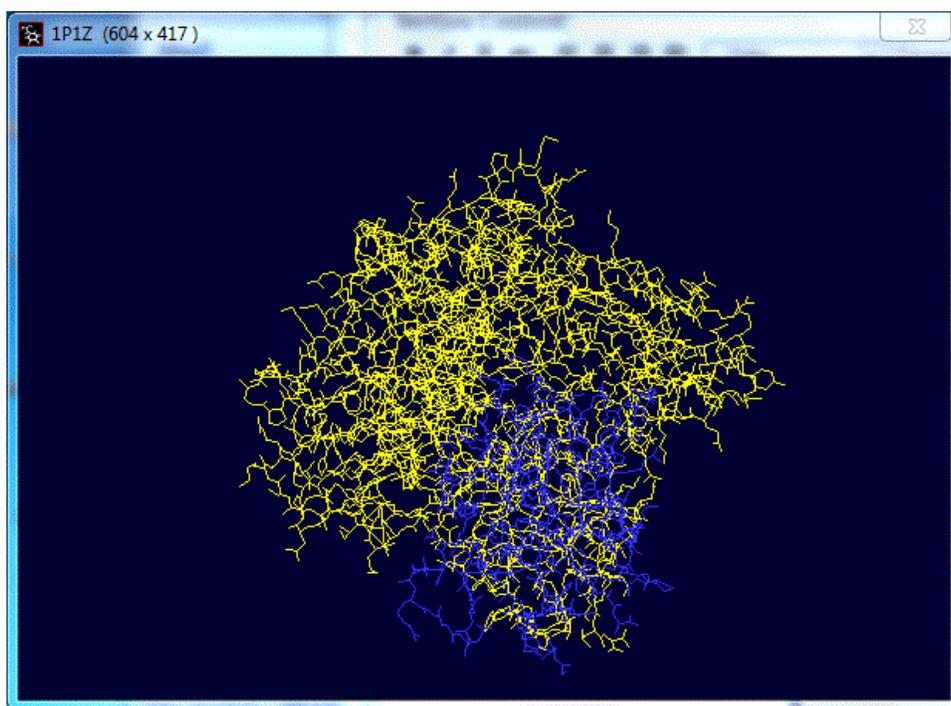
To make the two structures more easily viewed, remove the other chains from 1P1Z from the view and change the rendering to ribbons. You can do this from the control panel by selecting only chain D from 1P1Z, then selecting ribbons for both structures.

Then you can select **Improve Fit** from the **Fit** menu. Now you can see that some of the major structural features (beta strands and alpha helices) are aligned.
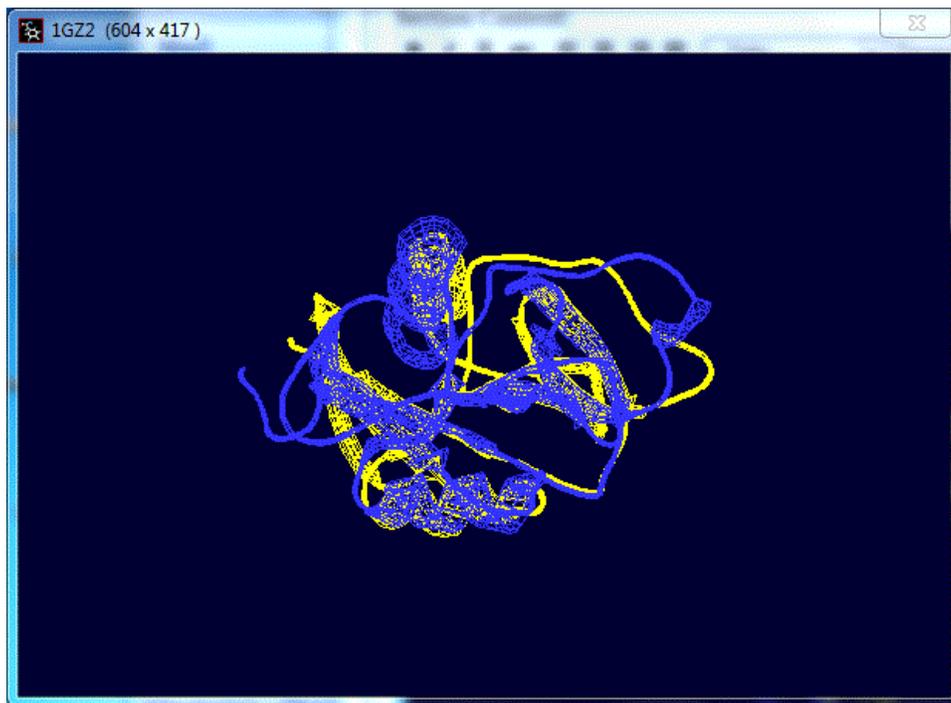
You can use the many options from the other menus to explore your structure.

Open the sequence alignment window by clicking on the **Wind** menu, then selecting **Alignment**. This way you can see residues selected in both the sequence and the structure.

- Use the **Select** menu to highlight accessible residues, neighbors of a specific residue, protein clashes and many other options
- Use the **Build** menu to add residues, remove residues, break or ligate a backbone (especially useful when you are mutating residues and exploring alternate backbone torsion angles), build loops and more.
- Use the **Tools** menu to measure energy, electrostatic potential or molecular surface
- Use the **Color** and **Prefs** menus to specify coloring or rendering preferences
- Use the **SwissModel** menu to upload a sequence to model against a structure, work with that model, or submit a model prediction job to the SwissModel server for a more computationally rigorous structure model prediction.
- Use the **File** menu to save an entire project as a .pdb file, so you can open it with other structure viewers, or come back to it to continue your work

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Other Structure Viewers

Many other excellent structure viewers are available for free download by users.

- RasMol has an open source version that all users can download. It produces colorful but slightly lower quality visualizations than some other viewers.
- Jmol is a Java-based structure visualization application that is very user-friendly.
- VMD (Visual Molecular Dynamics) is an extremely powerful structure visualization application that allows for a great deal of computational analysis.

- PyMol - the popular modeling software formerly free to all is available f**or a fee**

Resources and Help

Tutorials and help documents exist for PDB, Cn3D and Deep View.

- PDB's Education resources (PDB 101) page

- NCBI's MMDB help page
- NCBI's Cn3D tutorial
- NCBI's VAST help page

- Swiss PDB Viewer (Deep View) tutorial

Tutorials and help pages can also be found for most of the structure viewers listed in the section above. They usually can be accessed from the home pages for the viewers.

Many of these structure viewers also have user wiki sites, which can be found on their tutorial pages.

You can also get assistance in using many of these viewers from the Biosciences & Bioinformatics Librarian.