CCP4 Molecular Graphics Tutorials

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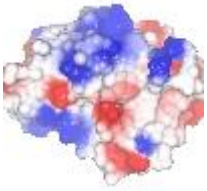
These tutorials are also available as a PDF file: .../ccp4mg/help/tutorials.pdf

A Guided Tour of the Program

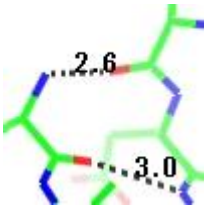
It is recommended that you follow the Introduction tutorial but you can pick and choose from the subsequent mini tutorials. They will probably take about ten minutes each.

Introduction - loading and viewing PDB or mmCIF files. Essential reading.

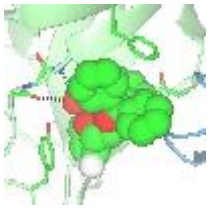


Surfaces - selecting and colouring and electrostatic surfaces

Superpose proteins - instamagic protein superposition

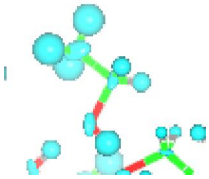


Investigating a structure - HBonds,Contacts,Solvent Accessibility,Geometry, Distances

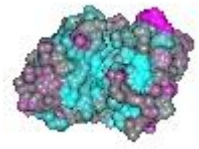


Ligand Binding Site Selection

Customised Atom Colouring



More Model Display Features

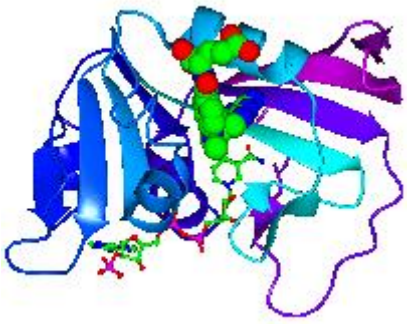


Importing Model Analysis Data

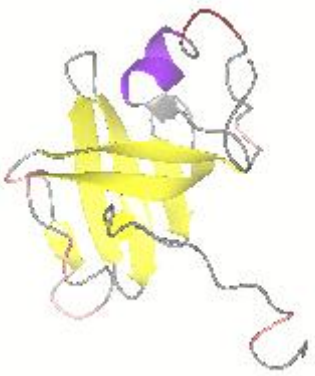
Electron density maps - better representation for images and packing diagrams

Adding Text and Extra Images

Creating publication quality images



Creating movies



Displaying and recording animations

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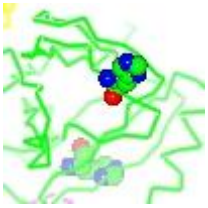
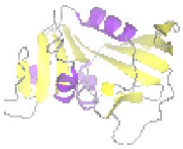
More Advanced Tutorials



Using the Selection Language



CCP4 Molecular Graphics Tutorials

Introduction - loading and viewing a PDB/mmCIF files

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The Picture Wizard

Starting CCP4mg

This may depend on your installation but..

Windows: click on the ccp4mg icon in the desktop.
Linux: type **ccp4mg** in a terminal window.
Macs: open an X11 terminal window (to do this load the X11 application and choose **Terminal** from the **Application** menu). Then type **ccp4mg** in a terminal window.

Two windows should appear: the large black 'main' window and the small white 'Display Table'. The top menu bar in both windows is the same and either can be used.

Copying some data to your own area

Some data files are provided which you should copy to your own area. Or you can try using your own PDB or mmCIF files and MTZ or CCP4 map files.
From the **File** pull-down menu select **Tutorials** and then **Get tutorial data**. You will be told that a directory called *ccp4mg_tutorial* has been created in your home area.

Assigning a project directory

CCP4mg understands the project directories as used by CCP4i. It is not essential to use project directories but they will help to organise your work. From the **Project** pull-down menu select **Edit Projects**. (If you get any warnings about locks, choose the 'Override lock' option). A window appears which lists the known project directories - to add a new one click on the **Add project** button. A new line appears with two entry fields - in the first field enter a short one-word name for your project such as 'tutorial' and then click the browse button and use the file selector window to select the *ccp4mg_tutorial* directory. To make this new 'tutorial' project the current working project click on the menu in the **Project for this session of CCP4mg** line and select 'tutorial' and then click the **Apply&Exit** button at the bottom of the window. You will be told that extra directories and files are being created in the project directory - these are for CCP4i (and, in future, CCP4mg) to keep track of your work.

Loading a PDB/mmCIF file

From the file pull-down select **Read coordinate file**. The file selection should list the files in your project directory - select **1df7** or a coordinate file of your choice (preferably one containing ligands). Click on the **Select&dismiss** button.
Look in the Display Table window (if you have lost it then use the **Windows** pull-down menu and select **Display Table**). There is more about the display table soon but for now you might want to click on menu which initially says **Bonds** menu and change it to something prettier such as **Cylinders**.

Moving around the molecule

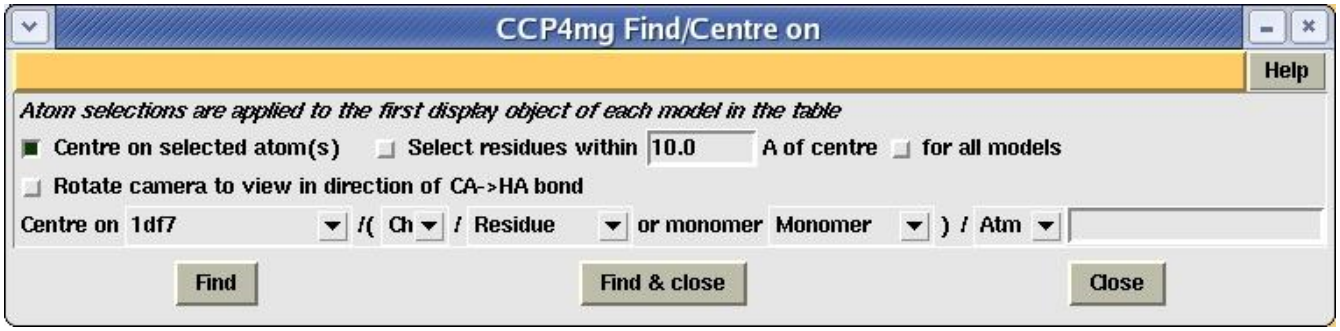
To rotate the molecule: with the cursor in the main window, hold down the left mouse button and drag

left-right or up-down. To rotate about the third axis hold down the shift key and the left mouse button and move mouse in circular motion.
To translate the molecule: hold down the middle mouse button and drag.
To zoom:hold down the shift button and the middle mouse button and drag up-down.
To centre on an atom: double click on the atom

More mouse and keyboard bindings

Finding things in the molecule

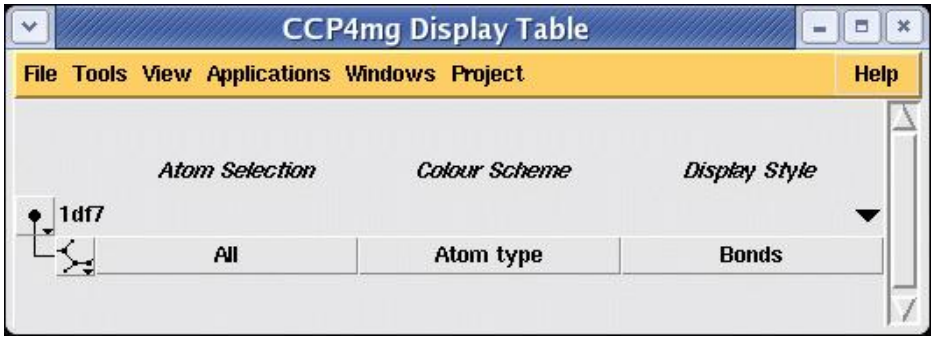
From the **Tools** pull-down menu select **Find/centre on...**.



A new window appears with several options at the top and then, on the line beginning 'Centre on',(going from left to right) menus to select a molecule, a chain, and a residue. Then there is then an option to select a monomer (that is a ligand) which is an alternative to selecting a chain and residue. And finally there is a menu to select an atom from the residue or monomer. Alternatively you can just type in the name of the model, chain, residue or atom that you want to find. The name is in the CCP4 atom naming format (see Interactive selection). For example try selecting the *NDP* ligand from the monomer menu and then click the **Find&close** button. The display should centre on the NADP ligand.

The Display Table

The display table lists all of the loaded data objects (for example each loaded PDB, mmCIF, MTZ or map file is one data object).



For each data object the display objects are listed one per line. You probably have one (1df7) data object and one display object currently listed. There are three columns in the table for the Atom Selection, the Colour Scheme and the Display Style of the display object.
Try some options from the Atom Selection menu (click on the button initially labelled 'All'):

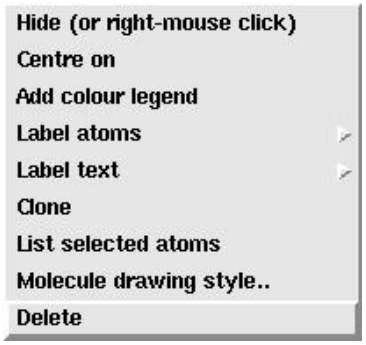
- **CA trace** - and then choose **..and monomers** and select a monomer such as *//501(MTX)* (or a ligand in your model).
- **Residue range ..** brings up a window in which you can select ranges of residues. Click on the **Add range** button to add a new line then you can either select a secondary structure element such as a helix or strand from the first menu on the left or select using the menu for the chain and residue. You can also select a residue from the display by clicking with the left mouse button on an atom in the display and then clicking with the middle mouse button in one of the text entry fields. Note that if you have something like 'CA trace' or 'main chain' selected then the atoms display will be only the CA atoms or main chain atoms of the range of residues selected.

- Select **Neighbourhood of..**. A window will appear, the top line of the window is similar to the 'Centre on' tool described above and allows you to select a chain, residue, ligand or atom. Try selecting the monomer *MTX* and click the **Apply&close** button. You will see just the ligand and neighbouring residues displayed.
- Select **Property..**. In the window that appears you can choose a property to select on (e.g. temperature factor, solvent accessibility) and enter some limiting value - try selecting all atoms with temperature factor greater that 20 (hint: the line looks like '20 < temperature factor').

Go back to having all atoms selected (and with and Display Style **Ribbons** looks nice) then try some options from the Colour Scheme menu (click on the button initially labelled 'Atom type'):

- **Secondary structure**
- **Blend thru model** and in the new window just click **Apply** to see the default colouring of the molecule from red to magenta from the N to C terminal.
- (Switch back to **Bonds** or **Cylinders** display style). From the Colour Scheme menu choose **Residue property** and **Solvent accessibility** to show the solvent accessibility of each residue.

To see what the colours mean you need the legend - to get this click on the icon on the left of the display object line which looks like  . This opens the display object menu,

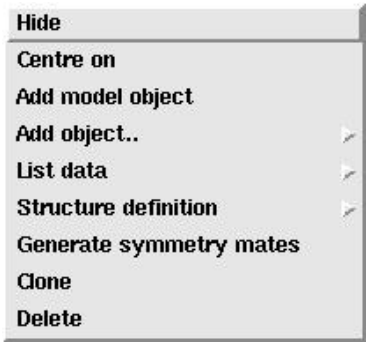


click the option **Add colour legend**.

Other options on the model display object menu to try are

- **Hide** which hides the object - click the menu again to get the option to **Show** the object. Note that when the object is hidden the icon is greyed out.
- **Label atoms** and select **One atom/residue** and then **Label text** and then click on the dashed line at the top of the menu to 'tear-off' the menu so you can select what appears on the label. Remove the labels by selecting **Label atoms** and **No atoms**.
- **List residue solvent access** (only available if you have the object coloured by residue solvent accessibility) will bring up a window listing the solvent accessibility and you can print the data to a file.

There is also a menu attached to the model object icon (currently ).



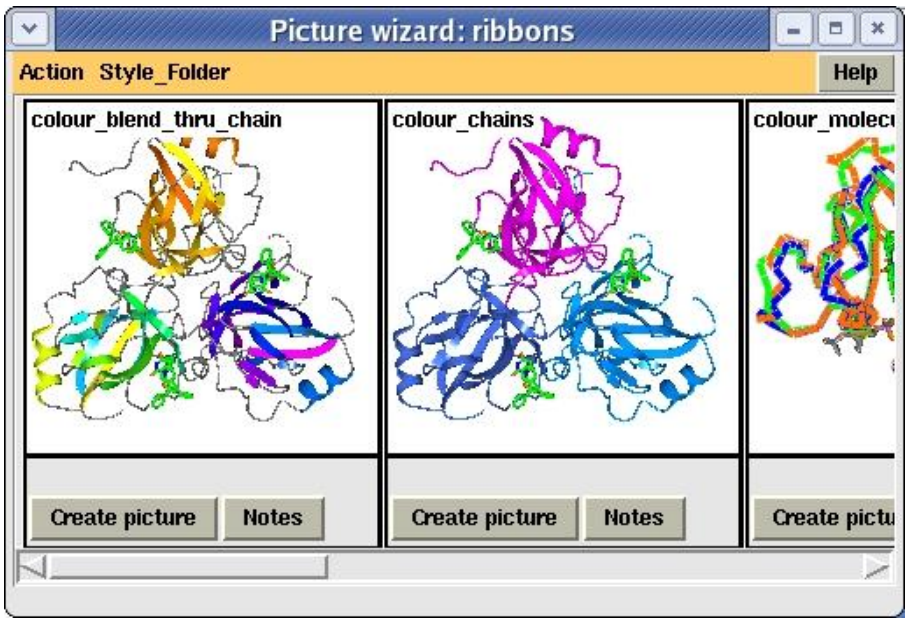
Try the options..

- **Add model display object** opens another line in the display table - this can be used to draw some part of the model in a different colour or display style - beware it is initially hidden; click on the greyed icon to make it visible.
- **Add display object** and try **Hydrogen bonds**, an additional row appears in the table for the hydrogen bond display object which atoms hydrogen bonds are drawn for and their appearance. For example, to see only the hydrogen bonds between the ligands and the protein select **..and monomers.** and **All** in the left hand column (the **Monomers only** should be on automatically) and select **All peptide** in the right-hand column.
- **Surface**The surface is not drawn immediately - you might want change the selected atoms covered by the surface to **All peptide** before clicking and clicking **Show** from the menu.

Finally, to delete the model look at the bottom of the model icon menu (that is the button) and select **Delete**.

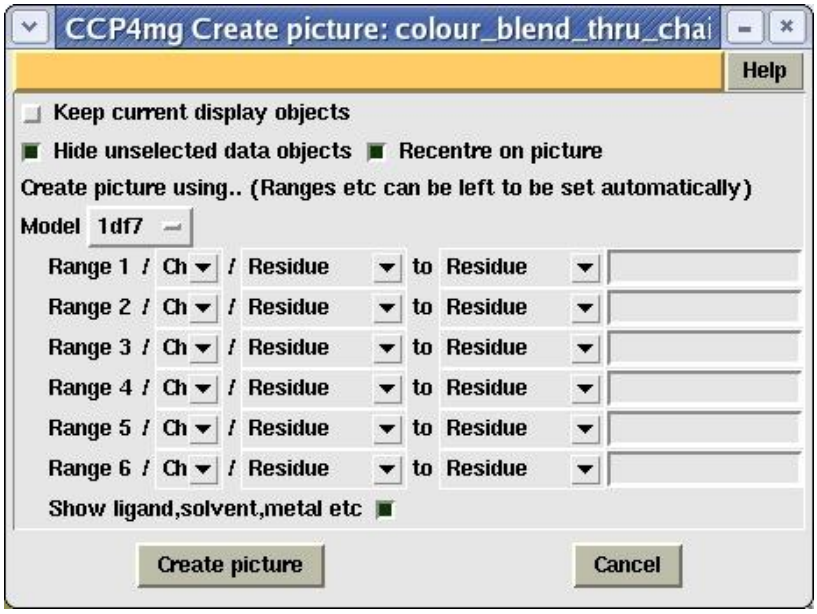
The Picture Wizard

And finally, the easy way to set up some standard pictures. From the **Applications** pull-down menu select **Picture wizard**.



In the new window, from the **Style folder** pull-down menu select **Ribbons**. You can scroll though a series of pictures and click on a **Create picture** button to draw your loaded model in the same style. You will usually be presented with another window with options to select chains or residue ranges to be drawn in the new style;

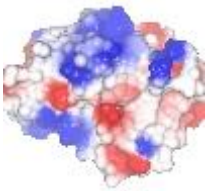
leaving these blank usually defaults to drawing the whole molecule in the new style.



Only beware, if you have more than one model loaded, that you select which model that you want redrawn. Click the **Create picture** button in this window to draw the picture.

The *ribbon* picture wizard styles will create one or more display objects for the protein drawn in ribbon style and then additional, separate display objects for any disulphide bonds, nucleic acid, ligands, metals or solvent that are present in the coordinate file.

Note also that at the top of the file browser (**File** menu, **Read coordinate file** there is a menu to choose **Representation style** which list the Picture Wizard style which can be applied to the model on loading.



CCP4 Molecular Graphics Tutorials

Molecular surfaces

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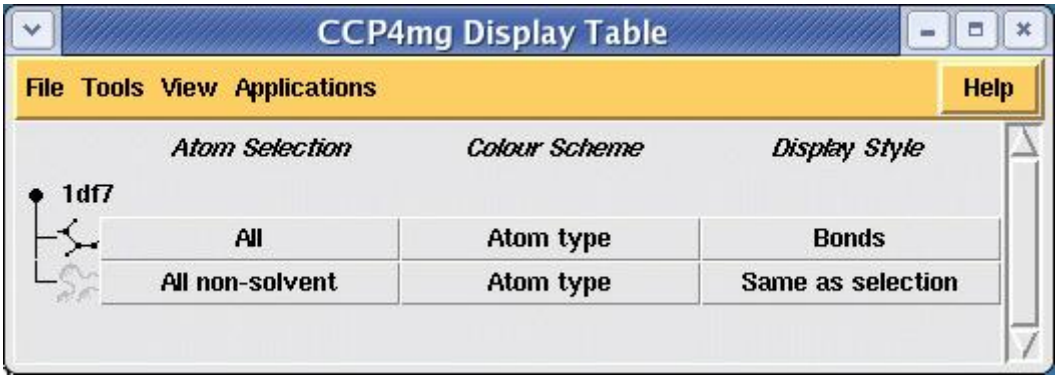
Creating and colouring a surface

Load a small protein such as *1df7* (small so calculations are quick). There are two ways to create a surface:

- In the Display Style menu of a model display object select **Surface**
- Click on the model icon (a dot next to the model name) and from the menu select **Add display object** and **Surface** to create a surface display object. This approach gives you more options.

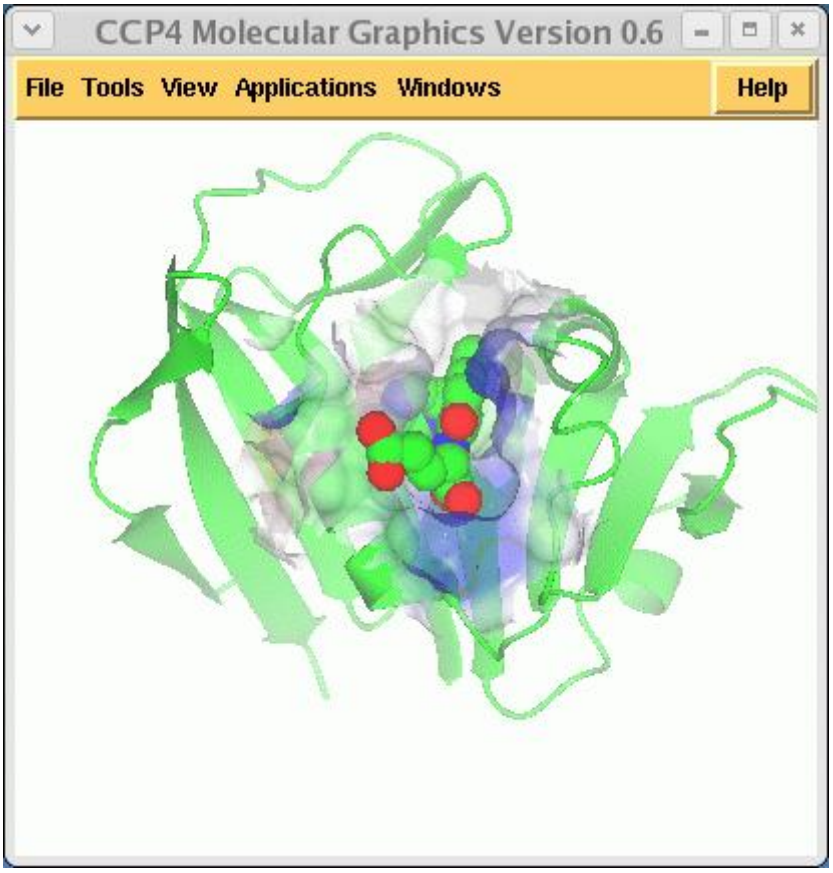


Calculating a surface may take a little time so when you create a surface display object it is not drawn immediately - you have the chance to select the atoms to be covered by the surface and then you should click on the surface display object icon  and select show.

Most of the items on the surface Colour Scheme menu are the same as those on the model colour scheme menu - the surface will just be coloured the same as the underlying atom. The extra option at the top of the menu are to colour by electrostatic potential (try it).

Covering a limited set of atoms

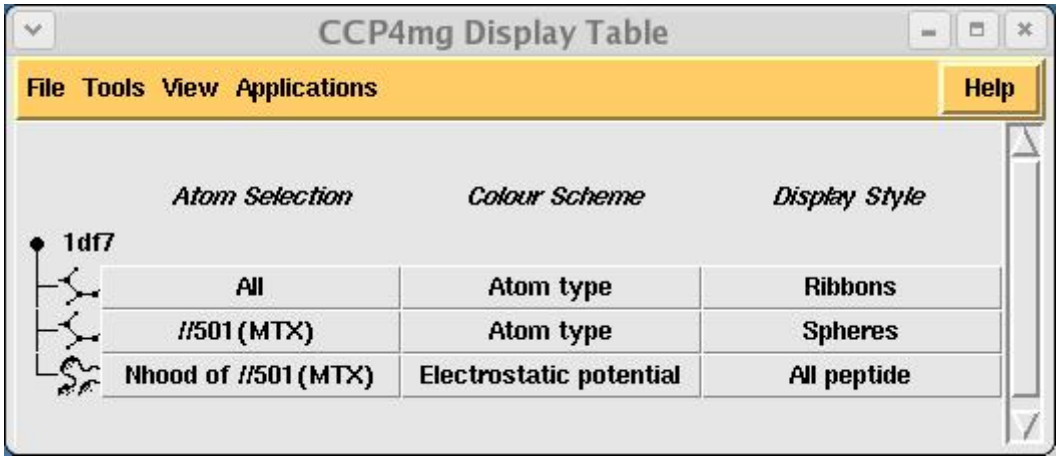
For example to create a transparent surface over just the binding site for the MTX ligand



First use the surface display object menu **Hide** the surface while we make two changes. Then select **Neighbourhood of** from the surface Atom Selection menu and in the top line of the window select the monomer *//501(MTX)*. Note that the selection radius is set quite high to 7A and that, by default, solvent and the named central atoms (that is the MTX ligand) are excluded from the selection. Hit the **OK** button. If you draw the surface now it will completely wrap around all of the selected atoms as if they were a single separate molecule. To prevent this go to the menu in the Display Style column to select the context for the surface and select **All peptide**. Now click on the surface display icon and select **Show**.

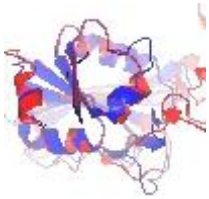
Click on the surface display object icon and select **Surface drawing style**. Try the various options. The opacity of the transparent surface can be changed by selecting **Set transparency** from the **View** menu, settting the opacity to say 0.5 for your surface object and then clicking the **Transparency on/off..** to on. The transparent surface is very slow to rotate so it is better to either hide the transparent surface or switch back to opaque surface if you need to rotate the model.

To get the image in the picture you need to set up ..



Notes

The calculation parameters and colour scheme for surfaces can be set in the **Preferences** window (find this at the bottom of the **Tools** menu).
More information on surfaces here.



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Superpose Proteins

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See general Superpose documentation

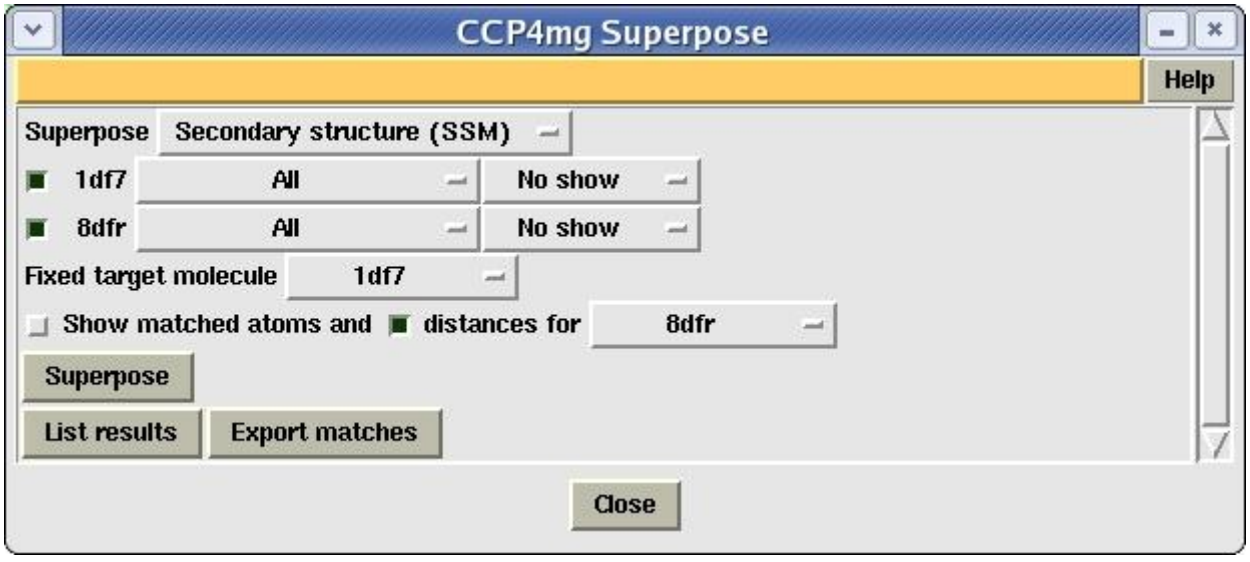
Load homologous proteins

Select two homologous proteins such as *1df7* and *8dfr* (hint to remove existing models: from the **Tools** menu select **For all data** and **Delete**).

To set the colour and display style for all models: from the **Tools** menu select **For all models** and **Appearance..** and in the new window set Colour to **By molecule** and Display style to **Worms** and then **Dismiss** this window.

Superpose

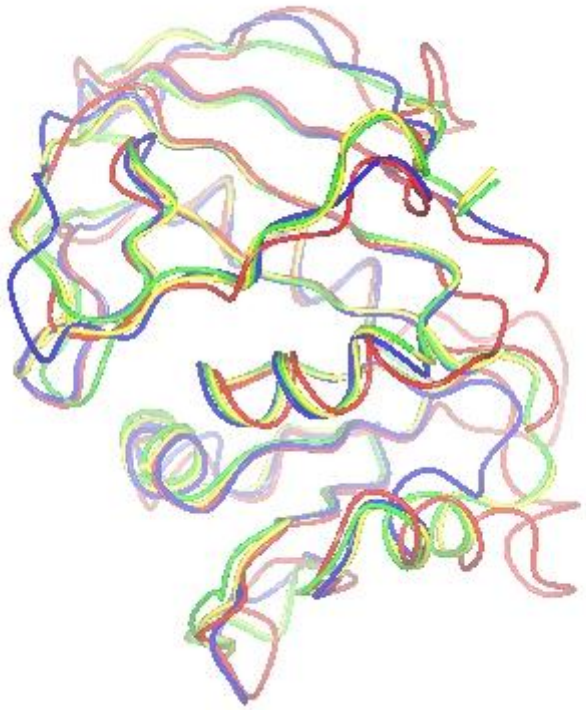
From the **Applications** pull-down menu select **Superpose**.



In the new window check that the Superpose mode (at the top of the window) is **Secondary structure(SSM)** and hit the **Superpose** button. The models will be superposed. To show the equivalent residues and distances between CA atoms toggle on the button labelled **Show matched residues..**.

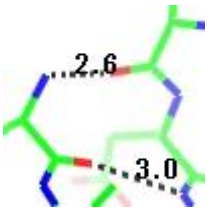
Multiple homologous chains

You can also try superposing the *4dfr* structure which contains two equivalent chains - if you want to treat these as two separate models load two copies of *4dfr* and in the Atom selection column for the first copy select **..of chains** and select chain A. Similarly select chain B for the second copy of *4dfr*. The Superpose proteins window should now list the two 4dfr models - for each of them click the button labelled 'All atoms' and select **As display object** and select the name of the chain. Now click the **Superpose** button.



Non-homologous proteins

This application will also make a good job of superposing non-homologous structures - it will overlay any similar pattern of secondary structure elements that can be found and the possible alternative matches can be reviewed.



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Investigating a Structure

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Geometry
Hydrogen Bonds
Solvent Accessibility Surface
Displaying vectors

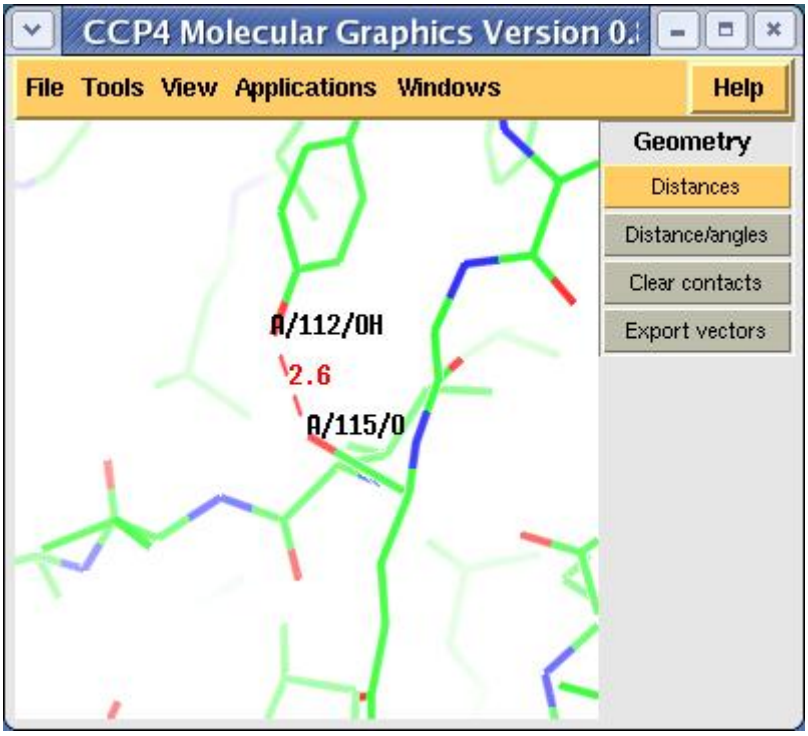
Introduction

Load any molecule of interest to you or use any one from the tutorial. It is easiest to work if the **Display style** is **Bonds** or **Fat bonds**.If you want to look at two or more homologous structures then the structures can be superposed - see the Protein Superposition tutorial. If you are looking at a new structure then some of the following selection and colouring tools may help you to familiarise

- Colour by **By chain** or **Blend thru model** and display style **Ribbons** to see the overall fold of the protein.
- Add another model object (to do this click on the dot menu and select **Add model display object**) and from the *Atom selection* menu select **..and monomers** (only present if there are ligands in the structure) and select **All** monomers. Change the *Display style* of these to something distinctive such as **Cylinders** or **Ball and stick**.
- If the structure contains multiple NMR models, nucleic acid or alternate conformations then options to select these features will be on the *Atom selection* menu.

Geometry

This section introduces some basic tools for interrogating the structure. From the **Application** menu select **Geometry**. A panel appears on the right side of the display window with a section titled 'Geometry'.



Try clicking on the **Distances** option and then, with the left mouse button click on pairs of atoms in the structure to show their inter-atomic distance. Note that the *Distances* button is highlighted in gold to show it is the active tool and the cursor is a cross to indicate that any atom picks will be used by the active tool. Now try clicking on the **Distances/angles** tool. A new window appears that will list the distances and angles between picked atoms. Pick a series of atoms and look at the information in the window.

Try clicking on an atom with the right mouse button and select the option **Contacts around this..** and **residue** which will show close contacts around the selected residue (note that there might not be any close contacts). The cutoff distances for close contacts can be changed in the *Geometry* applications *Preferences* window which can be accessed by clicking, with the RIGHT mouse button on the **Geometry** title and selecting **Preferences** from the menu.

The contacts and distances can be cleared from the display by clicking the **Clear contacts** button. Individual contacts can be deleted by clicking on the contact dashed line with the right mouse button and selecting **Delete contact**.

If you want to include the contacts in an output image you may want to have more options on display style. This is possible if you export the contacts as vectors using the **Export vector** button - see Displaying vectors

Hydrogen Bonds

To display the hydrogen bonds within the loaded model click on the dot icon next to the model name and from the menu select the **Add display object..** option and from the sub-menu select **Hydrogen bonds**. Note also the **Close contacts** option on the same menu that has a very similar interface to the hydrogen bond interface that we are about to look at. Now all hydrogen bonds within the structure are displayed and, in the display table, an extra line appears under the model name. This line has an icon HB , if you click on this one of the menu options is

Label - select this and the sub-menu option **Label bond lengths**. From the same menu you can also select **List/Save to file** and a new window will appear listing all of the hydrogen

bonds.

Several tools create similar windows; for example listing close contacts, secondary structure and the solvent accessibility. A couple of features of these windows are worth noting. Firstly, you can click on the **Save to file** option at the bottom of the window to save the listing to a file. Secondly if you click on an atom name (with the left mouse button) then that atom will be labelled in the main display window and if you double click on an atom name then the view will change to zoom in on that atom.

It is possible to display only the hydrogen bonds between two specified sets of atoms. The two sets of atoms are controlled by the menus in the *Atom selection* and *Display style* columns of the table. By default the atom selection is 'All'; click on this and change it to **Main chain**. The second set of atoms remains 'Same as selection' so only HBonds between main chain atoms are shown. Now try changing the 'Same as selection' to **Side chains** to see all HBonds between main chain and side chain atoms.

The criteria for HBonds can be changed in the **Preferences** window (on the **Tools** pull-down menu) - look in the **Model analysis** folder for **Hydrogen bonds**. The algorithm and parameters are explained in the Structure Analysis documentation.

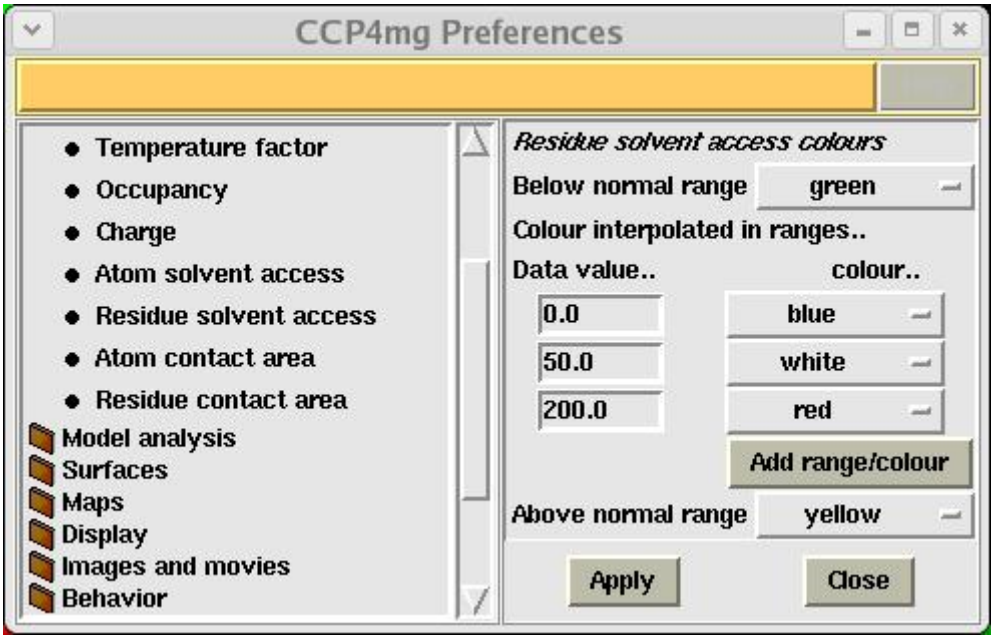
If you want to include hydrogen bonds when creating an image you may want to have more options on display style or to be able to add or delete some bonds. These things are possible if you export the hydrogen bonds as vectors - see Displaying vectors.

Solvent Accessibility Surface

The solvent accessible surface area is the surface area that is accessible to a 'water molecule'. In calculations the 'water molecule' is usually represented by a sphere of about 1.4Å radius (see Analysis documentation). To colour a model by the SAS area: from the *Colour scheme* menu select **Residue property** and then **Solvent accessibility**. There may be a short pause for the calculation and then the model is coloured with mostly blue on the inside of the model and red residues on the outside of the model. To see a colour legend click on the display object icon menu  and select **Add colour legend**. A legend appears at the bottom of the screen and an extra line also appears in the display table; it represents the legend object that can be manipulated in the same ways as any other legend object (for example click on the dot menu and select **Delete**).

Another option on the display object icon menu  is **List Residue solvent access**. This will open another window listing the solvent accessibility of residues and atoms. The data can be saved by clicking the **Save to File** button. Also try double clicking, with the left mouse button, on any atom or residue name; the display will recentre on the atom or residue.

The parameters for the SAS calculation can be changed in the **Preferences** window (on the **Tools** menu); open the **Model analysis** folder and select **Solvent accessible surface**. There is little reason to change these but you may want to change the colour coding. To do this open the **Model colours** folder in the **Preferences** window and select **Residue solvent access**.



The window has a table showing the parameter value and the colour for that parameter value. Every residue on the display is given a colour, dependent on its SAS, which is interpolated from the fixed values and colours in the table. If a residue SAS falls outside the normal range of values in the table then it is given one of the colours, specified at the top and bottom of the window, for below or above the normal range. The 'outside normal range' colours are usually contrasting the normal colours in order to draw attention to outliers but they could be made the same as the normal range colours. Note that any solvent in your model is coloured green (or the below normal range colour) because it is usually excluded from the SAS calculation and assigned a value of -1.0.

Note that there is also an option to colour by atom SAS: from the *Colour scheme* menu select **Atom property** and then **Solvent accessibility**.

Displaying vectors

Generate a vector file by either

- In the *Geometry* application, when you have some contacts displayed, click the **Export vectors** button
- Click on the Hbond display object icon HB and select **Export vectors**

In the file selection window enter the name for a vector file and make sure that the **Load vector file** button (at the top of the window) is clicked on. When you click the **OK** button the display window should not change significantly but a new vector object should be listed in the display window. The contacts or HBonds have been written to a file and then that file has been loaded and displayed in a similar style to the original data. To avoid confusion with the original data either

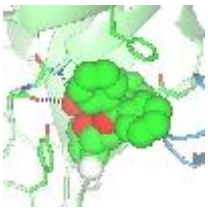
- Close the Geometry application by clicking with the right mouse button on the **Geometry** title and selecting **Remove** from the menu
- Click on the HBonds icon menu and select **Delete** from the menu

Now look at the new vector object in the display table and click on the middle column, labelled *Line style/colour* (the button is probably labelled 'red dashed' or 'white dashed') and try various

options from the menu changing the **line style** and **line colour**. For example style **dashed cylinder** works well if your model is displayed as cylinders or ball and stick. You may want to change the **cylinder radius** and **dash length**.

Also try changing options on the *Label style/colour* menu.

After you have changed the appearance of the vectors it is advisable to save the changes to the vector file. (Note that, unlike say model coordinate files and map files the vector file can contain information on how you would like the data to be displayed). To save the file click on the dot and select **List/save to file** from the menu. A new window will appear listing the vectors and their appearance (the format is explained in the Vector documentation). Click on the **Save to File** button at the bottom of the window to save this listing.



CCP4 Molecular Graphics Tutorials

Ligand Binding Site Selection

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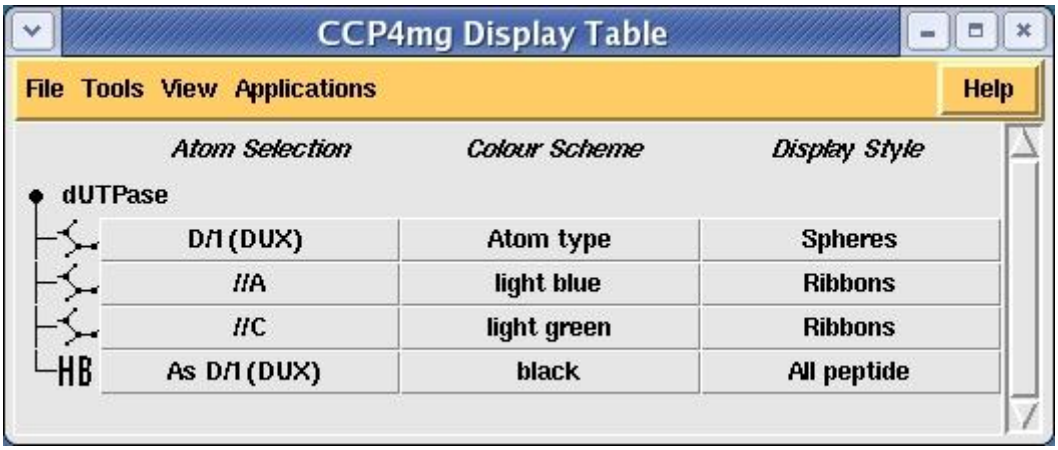
Copying selection to another model
'Neighbourhood' to select active site residues
Interactive selection
Picture Wizard
More complex selection tools using the selection language are described in the Selection language tutorial.

Introduction

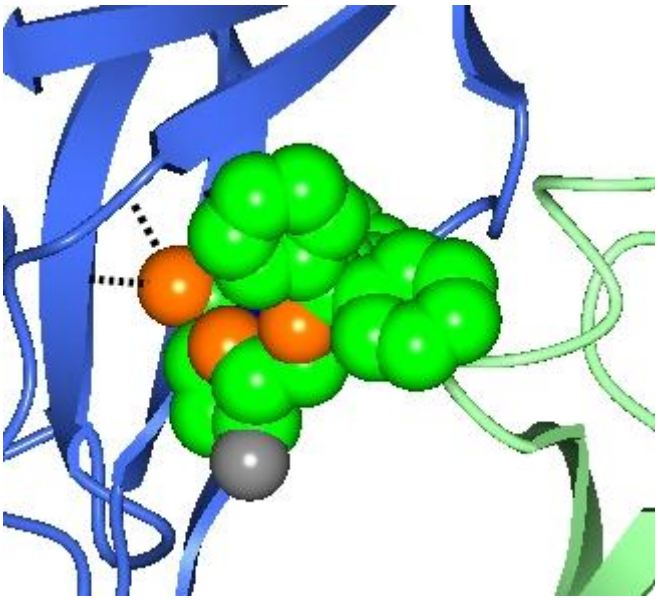
Making pictures can take a lot of time and much of that time is in selecting what to include in the picture and choosing the colouring - using the programs selection tools effectively can help save a lot of that time. The representation of a model is built up from several model display objects. All of the atoms in one display object must obey the same colouring scheme rules and will have the same display style (e.g. 'ribbons' or 'cylinders'). This tutorial is complementary to the Colouring tutorial. The quickest way to set up a complex picture is using the Picture Wizard, which creates the display objects for you but this tutorial explains the background for customising the Picture wizard pictures.

Simple menu-based selection

Load *dUTPase* (with the Representation style in the coordinate file selection window set to **All atoms**) and try to create a picture of the ligand binding site of one of the three homologous ligands. Create additional model objects by clicking on the model icon, the dot by the model name, and selecting **Add model display object**. Set up three model display objects; one for the monomer //D/1(DUX) and the other two containing the B and C chains. You can choose how to display and colour these objects but for example the setup



gives the image



The ligand D/1(DUX) is selected for the first object by using the **..and monomers..** selection menu item and selecting the D/1(DUX) from the submenu. The A and C chains are selected using the **..of chains..** selection menu item and selecting the appropriate chain from the submenu. Also shown here are the hydrogen bonds between the ligand and the protein by selecting **Add display object** and **Hydrogen bonds** from the model icon menu and then limiting the display to hydrogen bonds between two sets of atoms. The first set is selected in the first column of the hydrogen bond display object - choose the monomer *//D/1(DUX)* and the second set, selected in the third column, is **All peptide**.

Copying selection to another model

Load the model *1snf* which is a homolog of dUTPase. From the model icon menu (the dot next to the model name) select **Display same as** and **dUTPase**. The current display setup for dUTPase will be copied to 1snf. The 1snf has different ligands and so the display object selections which require the name of the ligand need to be entered again: for the first display object and the hydrogen bonds object select **..and monomers** and **//1170(UMP)**

In future we do intend to make the 'Copy from' tool smarter so it will recognise equivalent ligands and residues. You can delete or hide the 1snf model; it will not be used again.

'Neighbourhood' to select active site residues

Create another model object for dUTPase and, from the Selection menu, pick **Neighbourhood of**. A new window appears. In the top line of this window you select the 'central' atoms whose neighbours will be found. From the **or monomers** menu select **D/1(DUX)**. By default the selection group (fourth line of window) should be **residues** - change this to **main/side chain** so that if a side chain atom is close to the ligand all of the side chain is selected and if a main chain atom is close then all of the main chain of that residue is selected. Set **Radius** to 4.0 (Å). Click **Apply**. Make the display object visible and display style **Cylinders**. The side chains of the active site are displayed.

For your picture you may choose to add or remove some side chains or main chain atoms - the interactive selection tools, described in the next section, could be applied with the 'neighbourhood' selection as a starting point. But in the example below it is not used so make this display object invisible to avoid confusion.

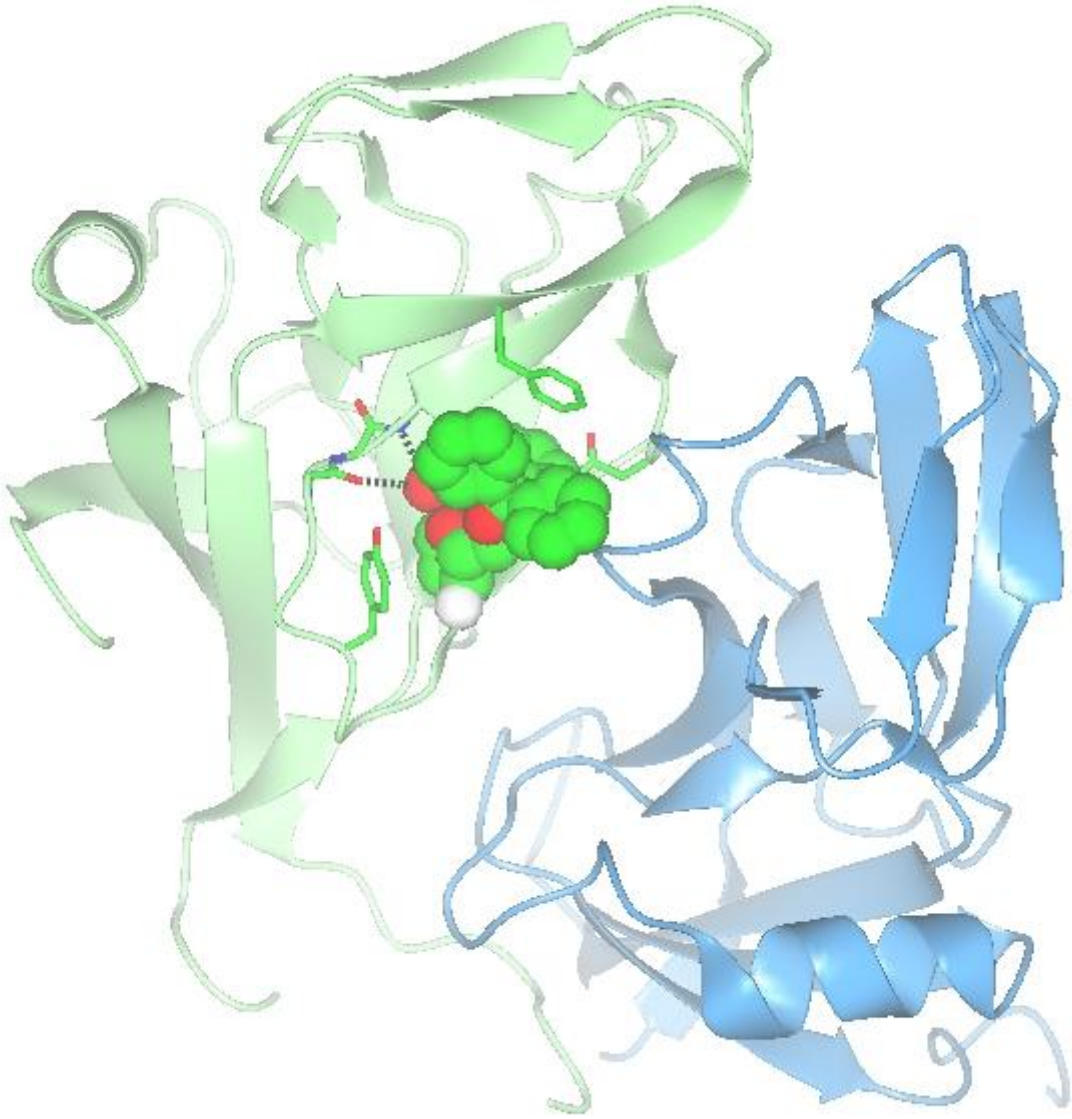
Interactive selection

To manually choose the residues of the active site create another model display object, make it visible and initialise the selection to no atoms by clicking **No atoms** on the selection menu. Then, from the bottom of the selection menu, pick **Interactive selection** and **Simple**. A new, temporary, object appears on the display which is a thin bonds display of all atoms in the model and you can click on items in this display to select them for permanent display. It is probably easier if you **Hide** the two ribbon objects for now. If you look around the ligand you will see hydrogen bonds to the main chain atoms of residues C/115 to C/117. To select this section of chain for display click on one atom in each residue with the RIGHT mouse button and from the popup menu pick **Select this..** and **main chain**. The selected atoms will be displayed with fat bonds. Other residues whose side chains might be selected are C/113(ASN) which forms a hydrogen bond to the ligand and C/112(TYR) and C/46(PHE) whose aromatic rings stack against the ligand. When happy with the selection go to **Interactive selection** again and switch off. The temporary thin bond object will disappear and the newly selected residues can be changed to a nicer display style such are **Cylinders**. The ribbons can be switched back on. A couple of final refinements..
the colour of the side chains can be set to the same colour as the C chain ribbon but check the option **Non-carbon by atom type** on the colour menu
the hydrogen bonds can be fatter - from the hydrogen bond icon menu 

select **Line width**

and set to 4.

A final image might look like this.



Picture Wizard

To create a similar scene automatically open the **Picture wizard** from the **Applications** pull-down menu. From the **Style folder** menu on the Picture wizard menu bar select **ligand binding site**. A series of ligand binding site scenes are shown; try the **site_and_ribbons** picture style by clicking on the **Create picture** button for that scene. A new window appears: make sure that the selected model is *pUTPase* and for the first ligand select D/1(DUX) then click the **Create picture** button. The scene in the display window will be redrawn; click the **Notes** button for the **site_and_ribbons** picture style to get an explanation of the picture.

CCP4 Molecular Graphics Tutorials

Atom Colouring

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Introduction
Changing the 'standard' colour schemes
Creating a customised colouring scheme
Colouring Hints

Introduction

Making pictures can take a lot of time and much of that time is in selecting what to include in the picture - using the programs selection tools effectively can help save a lot of that time. The representation of a model can be built up from multiple model display objects. All of the atoms in one display object must obey the same colouring scheme rules and will have the same display style (e.g. 'ribbons' or 'cylinders'). This tutorial is complementary to the Selection tutorial.

Load a model (for example try *dUTPase* from the tutorial data). It will look nice drawn as **Ribbons**. The model is a trimer with three bound ligands. Add another model object (click on the model icon, the dot by the model name, and select **Add model display object**) and for this object click on the *Atom selection* and select **..and monomers..** and select **All** to select all of the ligands. Click on the model display object icon  and select **Show** and also set the display style to **Spheres**.

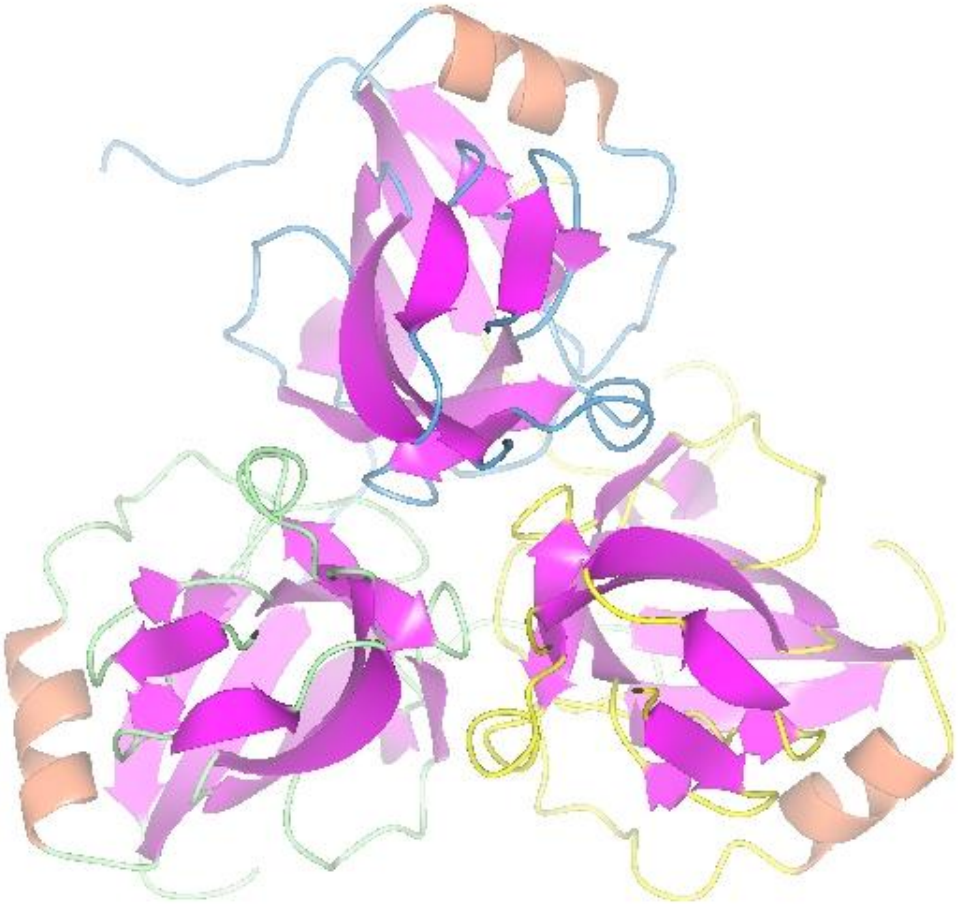
Changing the 'standard' colour schemes

The DUX ligand contains an atom of fluorine which is currently coloured white in the 'Atom type' colouring scheme. This could be changed by opening the **Preferences** window (from bottom of the **Tools** pull down menu) and selecting **Atom type** from the **Model colours** folder. To add a colour for fluorine click on the **Add range/colour** button and enter ' F' in the type column and choose a colour (I have used cyan). Close this window.

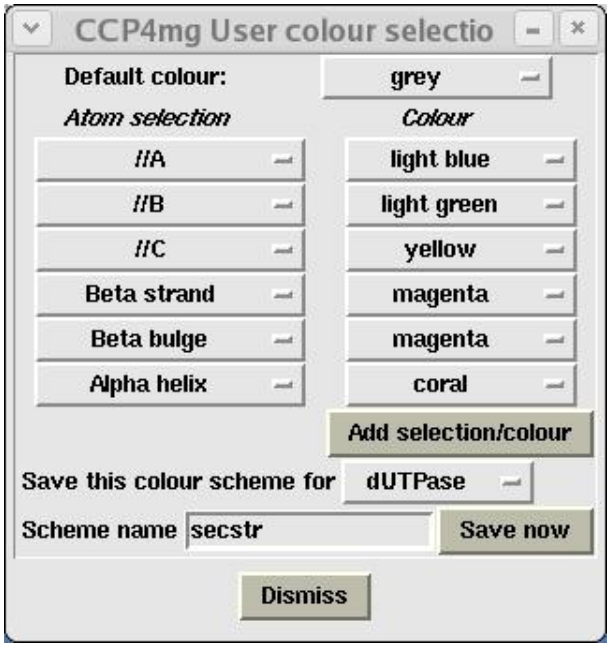
The **Model colours** preferences change the standard colour schemes which are on the *Colour scheme* menu for all models. The next section shows how to set up a novel colouring scheme.

Creating a customised colouring scheme

Models are loaded with the default colour scheme 'Atom type' - try changing this to **Secondary Structure** and then pick **Edit colour scheme..**. In the new window you can customise the colour scheme stating from the default colouring by secondary structure. For example you might want to set the Beta bulge which are currently green to the same colour as the beta strands and you may decide to not colour the different turns - these lines can be removed from the table by clicking with the right mouse button on either of the menubuttons in the line and selecting **Delete selection/colour**. Note that many tables in the interface have the same functionality on a 'right mouse menu'. You can also change the colours of course. Then to save your colour scheme enter a one word name in the **Scheme name** line and click on the **Save now** button. By default this colour scheme will only be available for the *dUTPase* model; the information is saved in a file called *dUTPase.ccp4mg* and is reloaded next time you load the same model. If you want the colour scheme to be available for all models then click on the menu labelled **Save the colour scheme for** and change to **all models**. If you now **Close** this window and change the colour scheme to something else you can later restore the saved scheme using the **Restore colour scheme** option.



To create the image above with the loop regions coloured differently for each of the three chains you need to to put the rules for colouring the chains (e.g. 'chain A is coloured yellow') before the rules for colouring the helices and strands so in the **Edit colour scheme..** interface click on the line labelled 'beta strand' and use the 'right mouse menu' option to **Insert above** and create two new rows. Then click in turn on the buttons currently labelled 'No structure' and 'All atoms' and choose **..of chain..** and select chains **A**, **B** and **C** for the three rules and then select a colour for each of them. So the window looks like this



While the Edit colour scheme window try clicking on an atom with the right mouse button depressed. The menu which appears has options to reset the colour for the picked atom, residue or secondary structure element. Also try selecting the option **Residue range from** and then right-mouse click on another residue and select the **Residue range from *your first residue*** and select a new colour. The range of residues will be recoloured and a new line will appear at the bottom of the Edit colour scheme window showing the new colour rule for the range of residues; you can click on the selection button, which is labelled **Ranges etc.** and pick one of the options **Main chain**, **Side chain** or **CA trace** to limit the selection to these residues within the range.

If you want to change the defined colours or define new colours then either:

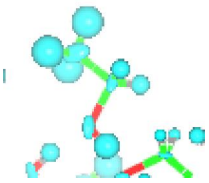
- Select **Interactive** from the bottom of one of the colour menus in the Edit colour scheme window
- Open the **Preferences** window (from the bottom of the **Tools** menu) and select **Colours** from the **Display** folder.

In the colour browser window choose the colour to change from the menu labelled **Define colour** at the top of the window or select **Add new colour** from the bottom of the menu and enter a name for the colour and hit the **Apply** button. To change the colour you can

- Use the sliders to set red/green/blue or hue/saturation/value
- Move the small square around the colour circle
- Click on the **Pick colour from screen** button and then click on a point on the screen

Colouring Hints

- If defining the colouring rules seems to be getting complicated it may be easier to split the displayed atoms between two or more display objects.
- Beware that pretty pastel shades are often washed out when projected and that the best contrasting colours can depend on the background colour.
- If you are making a series of images for a presentation or paper then try to be consistent in the colouring through all of the images.
- A colour legend may be helpful to an audience. See the tutorial on Legends and Annotation.
- In similar vein, also try to be consistent in the choice of views, and show or explain the relationship between views. Use the **Save/restore views** option from the **Tools** menu.



CCP4 Molecular Graphics Tutorials

More Model Display Features

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Download from structure database at EBI or RCSB
Thermal Ellipse

Download from structure database at EBI or RCSB

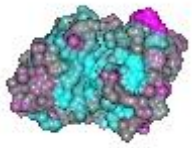
You need to be connected to the Internet. From the **File** menu select **Download coordinate file** and in the download window enter the 4-letter code for a model (e.g **1alz**). If you click return in the code window then a default name for the local PDB file is shown in the line below. Click the **Apply** button and the file will be downloaded to your computer and read into CCP4mg.

If you do not know the 4-letter code for the structure that you want then click on the **View server web page** button to bring up a web browser showing the structure database query page. Once you have found the structure you want you can use either the database download option or the CCP4 interface. If you have difficulty reading a file from a database then check that it is not a PDB file wrapped in an HTML file.

Thermal Ellipse

Load the model **1alz.pdb** or use any other coordinate file. Click on the model icon menu (the dot next to the model name) and select **Add display object..** and **Temp factor spheroid**. If the ellipse are not immediately displayed then click on the display object menu () and

select **Show**. By default the thermal ellipse are displayed as axes but they can be changed to solid using the menu in the right-hand, 'Display style', column.



CCP4 Molecular Graphics Tutorials

Importing Model Analysis Data

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(Mis)Using the PDB File Temperature Factor Column
List the PDB File
Labelling the atoms with the data values.
Colouring by 'Temperature Factor'
Selecting residues with a range of data values
Colouring residues with a range of data values

(Mis)Using the PDB File Temperature Factor Column

It is common practise for programs to output a variety of data to the temperature factor column of a PDB file - that is characters 61 to 66 of the lines beginning with the word 'ATOM'. CCP4mg will read such a PDB file and can display the data by various means. Load the PDB file *1df7_consurf.pdb* which contains the output from the ConSurf server for 1df7.pdb with the conservation of residues listed in the temperature factor column. The file pdb1df7.aln shows the sequence alignment for 50 homologous dihydrofolate reductase structures and the consurf value in the PDB file indicates the degree of conservation for each residue in structure. The lower the consurf value the more strongly conserved the residue. Listed below are some ways of viewing that data.

Since the non-peptide atoms do not have a consurf value and, in fact, still have the 'correct' temparature factor which might be confusing, exclude them from the display by changing Atom selection to **All peptide**.

List the PDB File

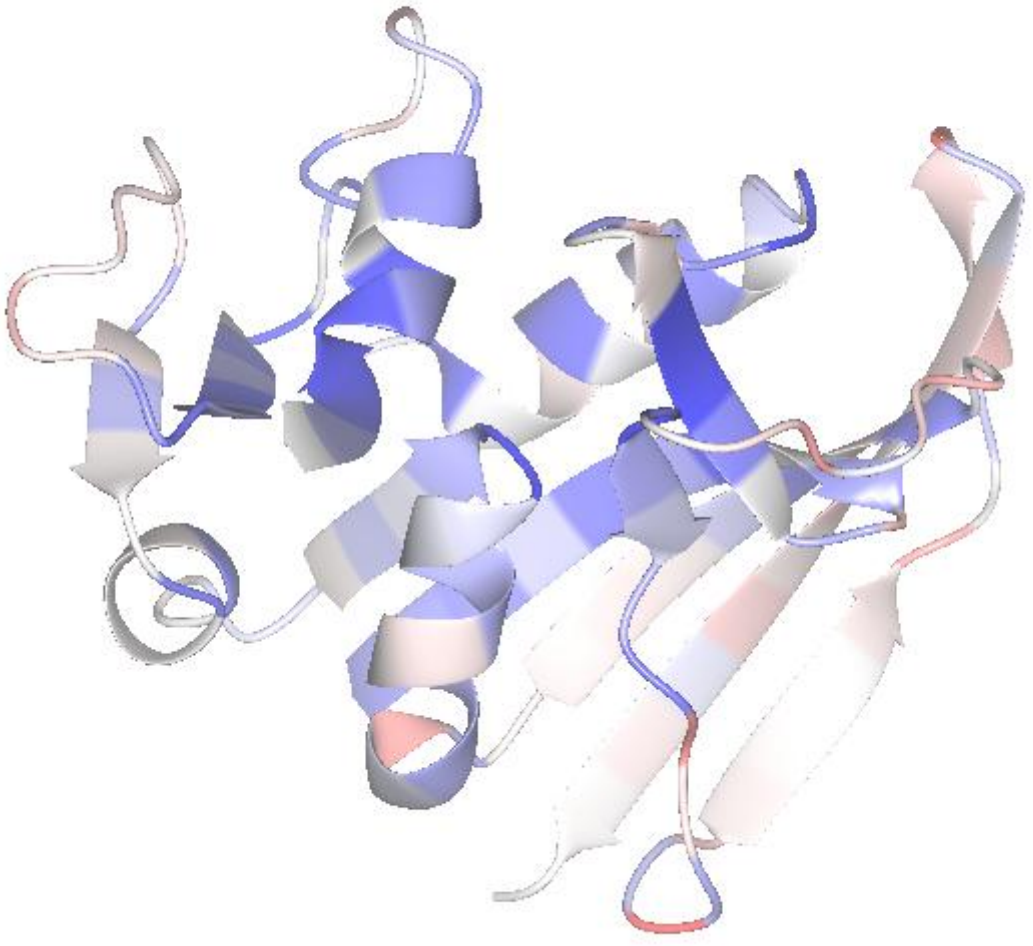
From the model data object icon menu (the dot next to the file name) select **List data** and **All atoms**. A window listing the PDB file appears. Scroll down to the lines which begin with the word 'ATOM'. Note that the 'temperature factor' values are the same for all atoms in one residue. To look at a particular residue in the file: double click (with the left mouse button) on one line in the file - in the main graphics window the display will focus on the atom that you have just clicked. Click on the **Close** button to close the listing window.

Labelling the atoms with the data values.

Click on the model display object icon menu  and select **Label atoms** and **One atom/residue** to label just the CA atoms (all the atoms in one residue have the same value). Then click on **Label text** from the model display object icon menu and click the dashed line at the top of the sub-menu to 'tear-off' the sub-menu into a separate window. Then click off the labelling of **Chain** and **Residue** (or whatever is currently on) and click on the labelling of **Temperature factor**. To switch off the labels: go back to the **Label atoms** menu and select **No atoms**.

Colouring by 'Temperature Factor'

From the Colour Scheme menu select **Atom properties** and **Temperature factor**. The model will probably be redrawn in green and blue in a way that is not very helpful because the values of the consurf parameter are not in the same ranges as usual temperature factors. The colouring scheme for the 'temperature factor' can be changed in the **Preferences** window (bottom of the **Tools** menu). Look in the **Model colours** folder for **Temperature factor**. Change the Data values for the colour ranges to be:
blue : -1.5
white : 0.0
red : 6.0
Also change the Interpolate mode to **between RGB values** - see colour interpolation. The peptide atoms will be coloured by blue to white to red depending on their consurf value of their residue. Non-peptide atoms are coloured yellow. If the model is drawn in display style **Ribbons** then it looks like this:



Selecting residues with a range of data values

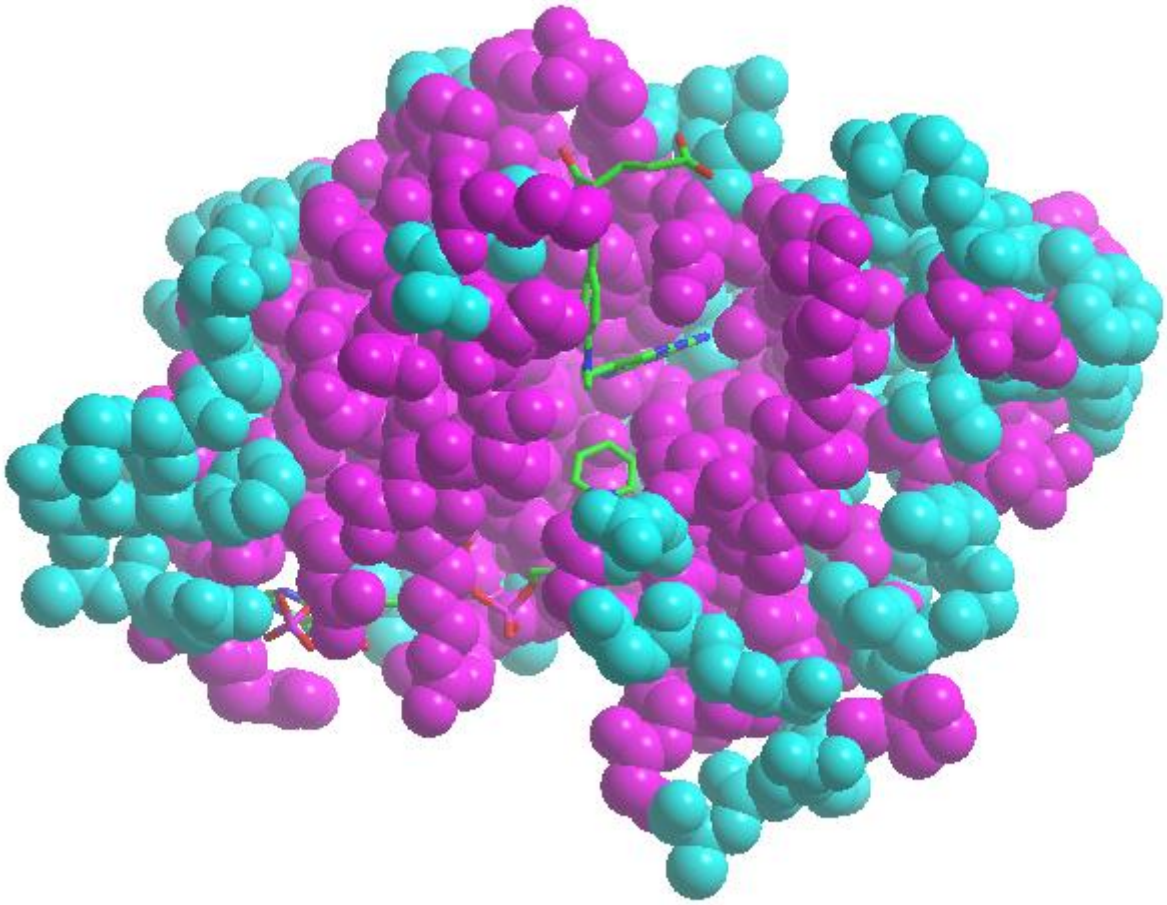
Restore the display style to **Bonds**. To select only those residues with 'temperature factors' in a given range of values select **Property** from the Atom Selection menu. The selection criteria is, by default, *Temperature factor* so you can just enter upper and lower range values in the two text boxes - for example enter '-1.5' in the lower range value and '0.0' in the upper range value and then click **Apply** to display only the conserved residues.

Colouring residues with a range of data values

In the previous example of colouring by 'Temperature Factor' the colours are blended between blue and white or between white and red. In this example the residues are grouped into ranges of data values and all residues within a given range are given the same colour.

Revert *Atom selection* to **All peptide**. From the *Colour scheme* menu select **Edit colour scheme..**. In the new window click on the **Add selection/colour** line a couple of times so that you have two lines in the window in which you can select two sets of residues and give them a colour. Click on the *Atom selection* button in the first row (labelled 'No atoms') and select **Property** from the menu and in the new window enter **-1.5** and **0.0** to select atoms with 'Temperature factor' (i.e. consurf values) in this range. Click on **Apply** and **Close**. Back in the *Edit colour scheme* window select a colour for these first set of atoms. Now select a second set of atoms with 'Temperature factor' values in the range **0.0** to **6.0** and give them a different colour. This has created only two groups - obviously you could create more. You can enter a name and save the colour scheme.

Displaying the peptide as spheres and adding another model object to display the inhibitor and cofactor as cylinders gives the following picture which shows the conserved residues, in magenta, around the ligand binding sites.



CCP4 Molecular Graphics Tutorials

Electron density maps

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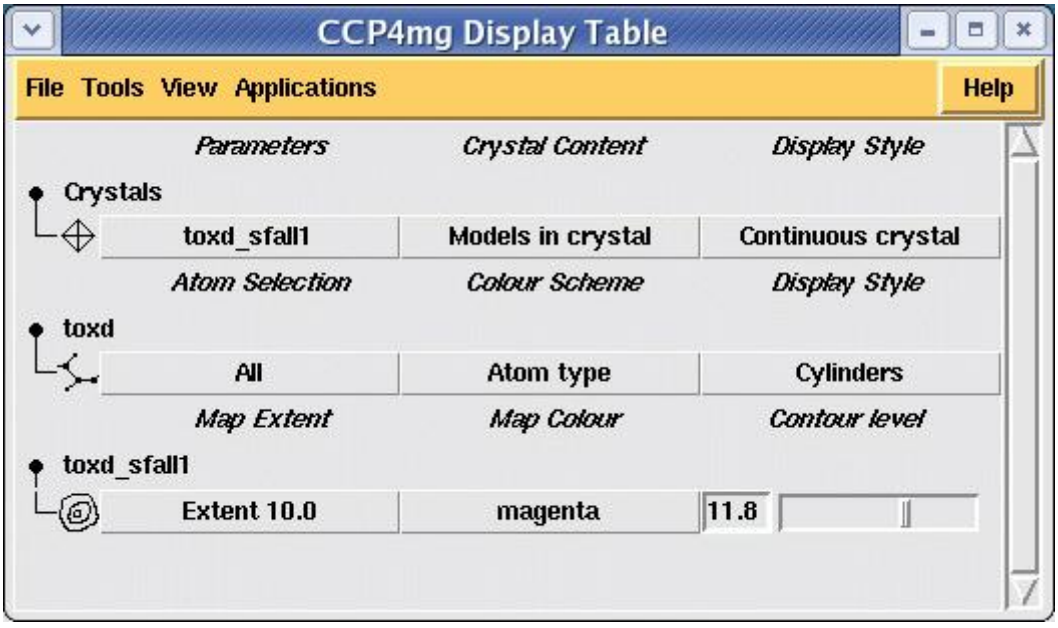
Loading a map and model
Better map representation for making images
Packing diagrams

Loading a map and model

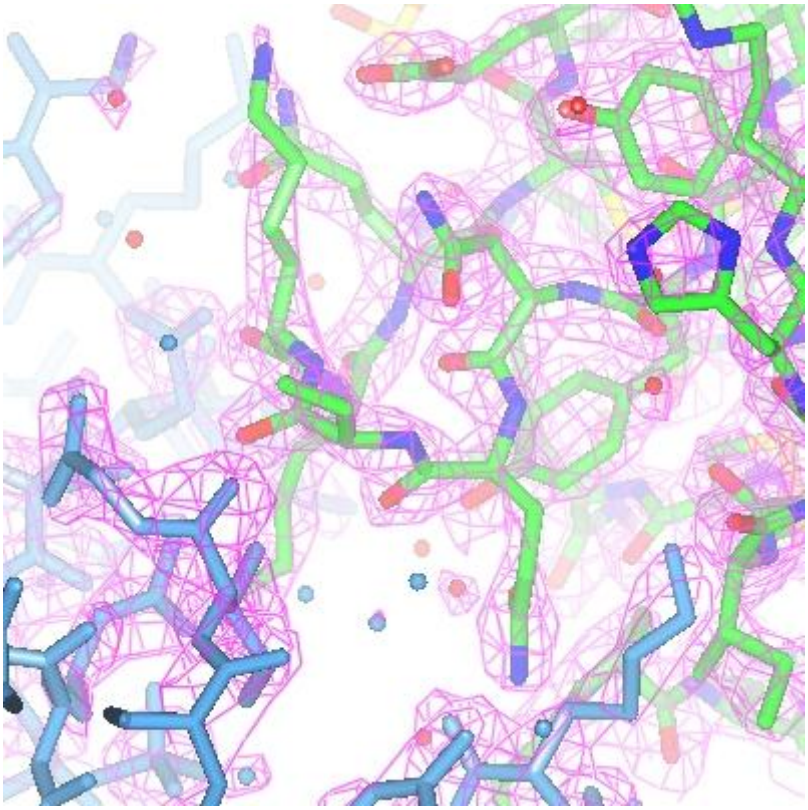
Load the coordinate file *toxd.pdb* and then read in either:

- A CCP4 map file: from the **File** pull-down menu select **Read map or MTZ file** and then **CCP4 map file** and select *toxd_sfall1.map*.
- A CCP4 MTZ (structure factor) file: from the **File** pull-down menu select **Read map or MTZ file** and then **CCP4 MTZ file** and select *toxd_sfall1.mtz*. In the new window you can select the structure factor and phase data from the file - accept the defaults by clicking **OK**.

The display table will then look like this:



There are rows for the loaded coordinate and map data and also a row for a *Crystal*. The display style is 'Continuous crystal' by default; to understand this try holding down the middle mouse button and dragging around the screen - the map will update automatically to cover the area at the centre of the screen and symmetry related models will appear when necessary. (If the symmetry models do not appear then look at the menu labelled **Models in crystal** and make sure that the *toxd* is set 'on').



For the map display object the Contour level has a slider which can be used to changed the contouring level. The scale is in an absolute scale of electrons/A3 but this can be changed to sigma levels (and other defaults can be changed) in **Map** options on the **Preferences** window (access this from the **Tools** pull-down menu).

Better map representation for making images

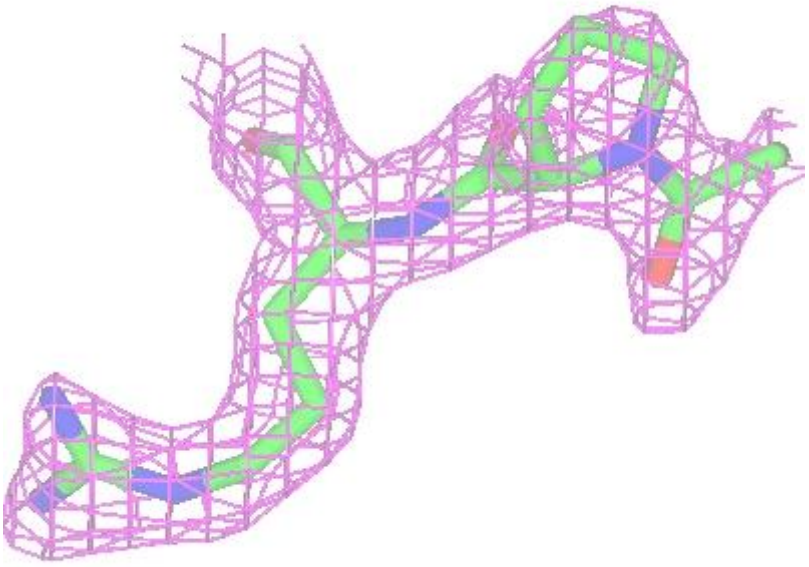
The map display style can be changed by clicking the display object icon , selecting

Surface style.. and then selecting an alternative to the conventional default chicken-wire style. **Cylinders** style is useful for creating distinct electron density maps for making images.

The appearance of the map can also be improved by reducing the map grid size. If you loaded data from a map file then the grid size is fixed in the file but if you loaded data from an MTZ file then try clicking on the map icon (currently a dot) and then select **Map grid size** from the menu. Try resetting the grid size to 0.5 - there will be a short delay whilst the map is recalculated.

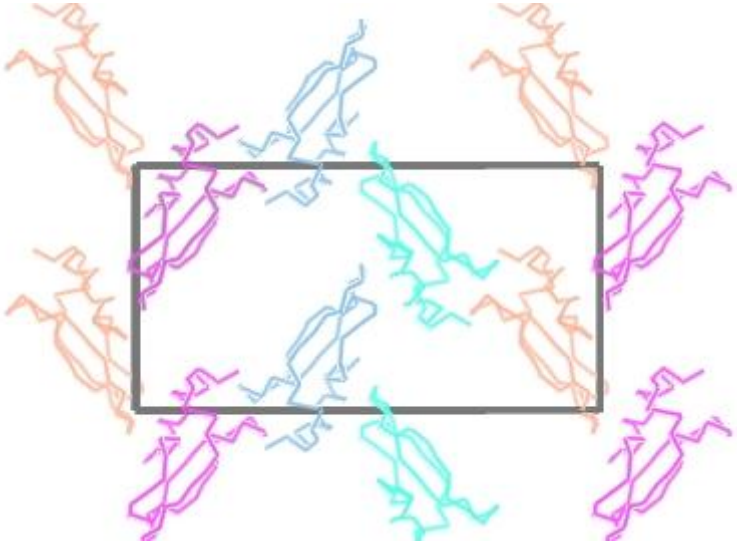
Another way to simplify an image is to show just the map around the features of interest and clip out extraneous density. To demonstrate this first create an new display object for the *toxd* model (click on the dot icon and select **Add model display object**) and then select a small number of residues for this object, for example by using the **..of residue ranges..** option and selecting a short range of residues. Displaying these residues in **Cylinders** style will improve the picture. You may need to find these residues on the display by choosing **Centre on** from the display object icon menu .

Now to display just the density around these residues click on the map Extent menu and select **Clip..** and **to toxd Ranges..**.



Packing diagrams

To show the packing of the molecule in the crystal first hide the map by selecting **Hide** from the map display icon menu and then change the *Crystal* Display style from 'Continuous crystal' to **Contents of one unit cell**. All the symmetry models necessary to fill a unit cell will be displayed. The **Cell edges** can also be toggled on from the *Crystal* Display style menu. The image may be clearer if you change the atom selection for the *toxd* model to **CA trace**.



CCP4 Molecular Graphics Tutorials

Text and Extra Images

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Entering Text
Moving Text
Adding Other Images

Entering Text

There are currently two types of text ..

- A 2D legend that can be placed anywhere on the screen and that will not move if the view is changed. To create a legend select **Add legend** from the file pull-down menu.
- 3D annotation on a model that will move with the model. To create annotation you must have a model loaded then from the model data menu select **Add display object** and then from the sub-menu **Annotation**.

The legend and annotation objects have many features in common - try these..
Click on the button labelled **Enter text..** to open a window with a simple text editor. Type in some text. Note that you can customise the text using the **Underline**, **Bold**, **Italic** buttons or **Colour** menu. Click the **Apply** button to display the text in the main graphics window. By default a legend is first positioned at the bottom left of the screen. Annotation text is by default placed at position 0.0,0.0,0.0. If you can not immediately find the annotation click on the icon  and select **Centre on** from the menu; this should change the view to centre on the text.

From the legend or annotation icon menu (click on ) select **Font** and try changing the font.

Probably the easiest way to add annotation to the display is using the tools in the Picture Wizard.

Moving Text

From the icon menu try selecting **Move object**. The icon is highlighted in gold to indicate that this is the active moving object. To move the text hold down the *Control* key and the middle mouse button and drag the text.
An alternative way to move a legend is using the sliders on the display table that control the x and y coordinate of the bottom left of the text. The extent of the screen is between zero and one with x=0.0,y=0.0 being at the bottom left of the screen.
An easier way to place annotation on a particular atom or residue is using the window opened by clicking on the button in the right hand column of the display table. In this window is the usual atom selection tool with menus to select a chain, residue, monomer and atom. Note that you could also 'cut-and-paste' an atom into the final entry box by clicking on the atom with the left mouse button and then clicking in the entry box with the middle mouse button. You must

then click the **Apply** button to move the text to the selected atom. If you select a residue or monomer then the text will be placed at the centre of that entity. While this window is open there is also the option to drag the text with the *Control* key and middle mouse button. Remember to rotate the view 90 degrees about the y (vertical) axis to look at the image 'from the side' to check the placement of the annotation in the third dimension.

Adding Other Images

CCP4mg can load and display images in PNG,GIF and JPG format. The image can be scaled and moved around the screen. This option might be useful for displaying a logo or, say, a graph.
From the **File** pull-down menu select **Add image** and select the file *weblogo175.gif*. The CCP4 logo will appear at the bottom left of the display window. The image is represented on the display table by a line containing three slider bars. The one on the left controls the image scale and the other two control its position. The image can also be moved by clicking on the 

icon and selecting **Move object**. Moving the image is then the same as for moving text as described above. Note that this image has a transparent background and this is probably a desirable feature for many images that you might want to display.

CCP4 Molecular Graphics Tutorials

Presentation graphics

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Things to consider before making a picture
Screen snapshot
Output Postscript
Reviewing Images

Note: If you have a packing diagram set up after the Maps tutorial then this is a good example to output in PostScript format so go here first.

Things to consider before making a picture

Once you have set up the picture on the screen things you might want to check:

- The appearance of ribbons, cylinders etc. can be changed in the **Preferences** window (accessed from the **Tools** menu); click on the **Model display** folder and choose **Drawing style**. If necessary you can set these drawing style parameters for individual graphical objects - from the model display object icon menu select **Molecule drawing style..**. Note that graphical primitives such as ribbons and spheres can be drawn at variable speed/quality (in **Preferences**, **Display** folder, **Render quality**) but when outputting an image the program automatically changes these to best quality.
- Is the background colour appropriate? Look at the **View** menu **Background colour**.
- Is the fog level appropriate? The depth queue fog can be toggled on or off from the **View** menu **Depth queue fog** or the fog level changed using the **Clip plane/depth que slider** option on the **View** menu to open a panel, at the bottom of the main window, with a slider controlling fog density.
- Usually the output image will have the same pixel resolution as the display window so choose an appropriate window size and ratio. Note that images to be put into printed publications need to be saved at much higher resolution such as 1000x1000 pixels which implies a bigger image. To get high resolution images it is recommended to save at 2 or 3 times the screen size (see later notes).
- When outputting an image file the program automatically saves the program status to a file with the image file name and the extension *.pkl*. If the image needs changing later the status file can be loaded via the **Save/restore** option on the **Tools** pull-down menu. A good reason for annotating images within CCP4mg rather than adding labels afterwards is that the annotation is saved and will not need redoing if the image is revised.
- In the **Preferences Images and movies** folder look at the **Screenshots** options. When creating an image file the program can take the picture directly from the screen or it can redraw the scene in an offscreen buffer and output the image from there. The disadvantage of taking the picture directly from the screen is that if any part of the display window is covered then what should appear there is lost from the output image. It is better therefore to use the back buffer but this may not work on all hardware. Another improovement is to smoothe the edges of ribbons and spheres etc. by anti-aliasing. This process takes a few seconds but produces a much neater result. Unfortunately this also may not work on all hardware. Ideally in the **Screenshots** options you should set the offscreen buffer and anti-aliasing on.

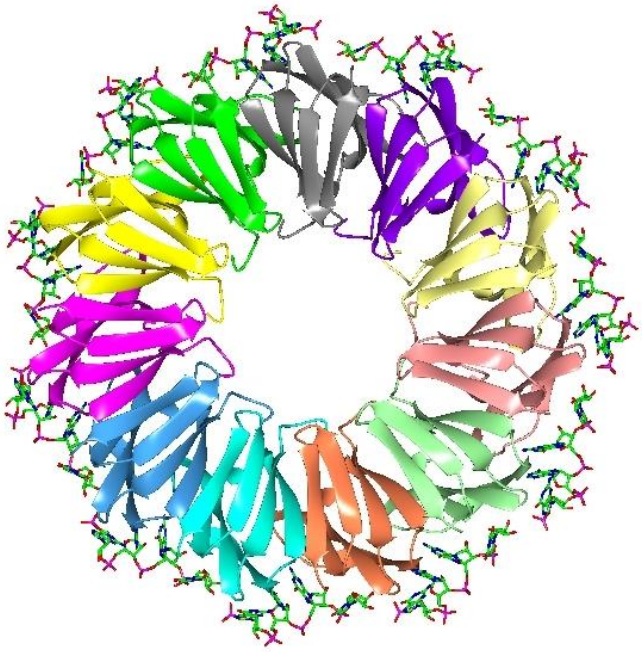
Screen snapshot

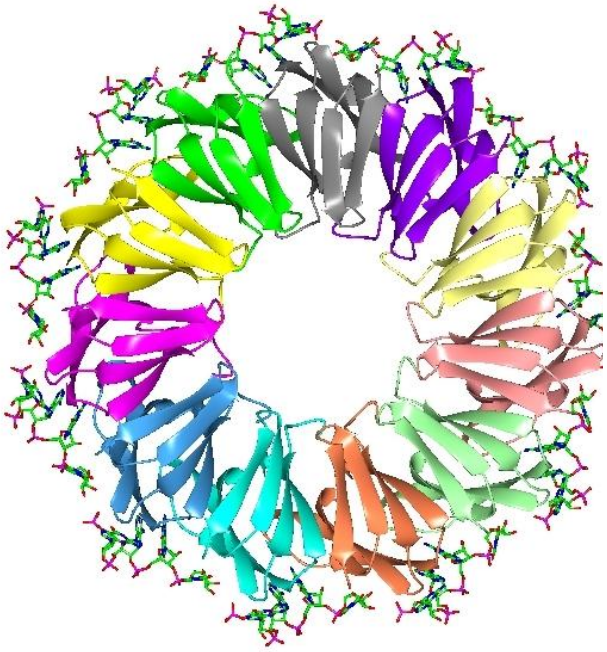
Set up any picture - if you have nothing already try loading *rnase.pdb* and choosing one of the ribbons representation styles from the top of the file browser window.

A screen snapshot can be output in a variety of formats; from the **File** menu select **Output screen image..** and **Screen snapshot** and select the required output file type from the menu in the file browser. Look at the options at the top of the file browser window - these can be used to set the resolution of the output image. Enter a file name and hit the **OK** button. There may be a short pause while the image is written out and then a web browser window should appear displaying the new image.

Now try again but in the file selection window click the button by **Display window size with magnification** to set magnification on and set the magnification to 2.

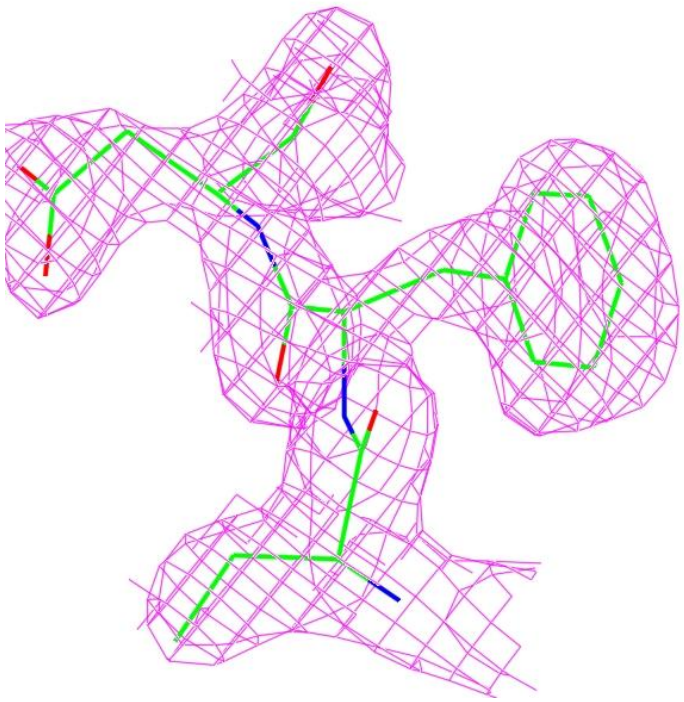
Also try creating a stereo image. Switch the screen magnification back to 1 and toggle on the **Make stereo picture** button and hit the **OK** button. This time three files will be created: *filename*_left.*ext* and *filename*_right.*ext* which contain the left and right eye view and *filename.ext* which contains a merged left and right eye picture.





Output Postscript

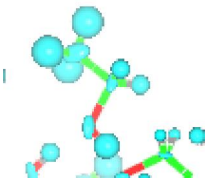
Postscript output works best for pictures which contain only lines such as models drawn in Bonds display style and maps in chicken-wire style but will reproduce these at very high resolution. Try setting up such a picture and output select **Output screen image..** and **Postscript snapshot**. The picture below is not actual Postscript because is will not work in web pages but the picture shows the sort of diagrams that are presented well by Postscript.



Reviewing Images

By default a newly created image will be displayed in your web browser. You can prevent this by setting the **Display image in web browser** option off the **Preferences** window (on the **Tools** pull-down menu, in the **Images and movies** folder.)

The following suggestions depend heavily on the setup of you computer.
To see the images that you have created try using the operating system file browser to select the image file which should be in the directory *ccp4mg_tutorial* which is in your home area. Under Windows this probably means C:\Documents and Settings*your_name*\ccp4mg_tutorial. The browser should choose an appropriate program to display the file but note that a Windows system might not have anything appropriate installed to view a PostScrpit file.



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More Model Display Features

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Download from structure database at EBI or RCSB
Thermal Ellipse

Download from structure database at EBI or RCSB

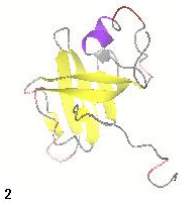
You need to be connected to the Internet. From the **File** menu select **Download coordinate file** and in the download window enter the 4-letter code for a model (e.g **1alz**). If you click return in the code window then a default name for the local PDB file is shown in the line below. Click the **Apply** button and the file will be downloaded to your computer and read into CCP4mg.

If you do not know the 4-letter code for the structure that you want then click on the **View server web page** button to bring up a web browser showing the structure database query page. Once you have found the structure you want you can use either the database download option or the CCP4 interface. If you have difficulty reading a file from a database then check that it is not a PDB file wrapped in an HTML file.

Thermal Ellipse

Load the model **1alz.pdb** or use any other coordinate file. Click on the model icon menu (the dot next to the model name) and select **Add display object..** and **Temp factor spheroid**. If the ellipse are not immediately displayed then click on the display object menu () and

select **Show**. By default the thermal ellipse are displayed as axes but they can be changed to solid using the menu in the right-hand, 'Display style', column.



CCP4 Molecular Graphics Tutorials

Animations

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Introduction
Viewing an Animation
Making a movie
See also Animation reference.

Introduction

This is an example of a morph which is a short animation that shows the transformation between two conformations; it is intended to help a viewer visualise the differences between the conformations and there is no claim that the intermediate steps represent a true conformational pathway. The tutorial directory contains a subdirectory *morph* which contains a series of PDB files which come from the morph server MOLMOV (Yale Database of Macromolecular Movements) and show a morph between two conformations of the NMR structure 1liz.pdb.

See an example here - morphing between two of the NMR models in 1liz.pdb done by MOVMOL.

Viewing an Animation

Delete any loaded models (from the **Tools** menu select **For all models..** and **Delete**) and then load the PDB file *ccp4mg_turial/morph/ff0.pdb* which is the first file of the morph. From the model icon menu (the dot next to the model name 'ff0') select **Animation** and **Select multiple PDB files..** and again select the PDB file *ccp4mg_tutorial/morph/ff0.pdb* - the program will now automatically select all of the other PDB files in the morph directory with related names. Now go again to the model icon menu and select **Animation** and **Run animation** to see the animation. It can be stopped by clicking the **Stop animation** button at the top of the graphics window or by hitting the keyboard **escape** key.

Now try creating a more complex picture - for example making the display style for the model **Ball and stick** and by displaying hydrogen bonds (from the model icon menu select **Add display object..** and **Hydrogen bonds**). And run the animation again.

Making a movie

There is a separate Movie tutorial and movie reference with more information but this section will show quickly how to record an animation. If you are making your first movie then from the **Applications** menu choose **Movies** and **New movie** and enter a name; a directory, *project_directory/movie_name*.ccp4mg_presentation will be created this is where images are stored and the movie will be put.

Now reset the conformation to the first step by selecting **Animation** and **Go to step..** and in the new window setting the step to zero. Make sure the model is suitably positioned in the

centre of the screen.

Now make a snapshot of the current display by right-mouse clicking on the frame in the movie window labelled **Insert next snapshot here** and select **Insert current view/display** from the pop-up menu. A small image of the current display should appear in the movie window. This snapshot is labelled 00001 (any subsequent snapshots will be labelled 00002, 00003 etc.). A movie scene will be created based on this snapshot; beneath the snapshot are the options for the scene. The time for the scene to run should be set automatically to accommodate one run through the animation. On the bottom line of this interface change the *Display* to **interpolate**. From the **Action** menu choose **Preview**; this should show, in the main graphics window, what will appear in the movie but will not actually record anything. It should run once through the animation. If you double the run time and **Preview** again you should see the animation run forwards and then backwards to finish on the initial frame. To actually make the movie you should select **Record** from the Action menu - this will save the screenshots that will make the frames of the movie. When this is finished select **Compile scene(s)** from the Action menu; this runs an external process to convert the individual frames into one movie file, when the process is finished the movie should be played automatically. The movie file will be called something like

```
...ccp4mg_tutorial/test.ccp4mg_presentation/scene_00001/movie.gif
```